

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> e fluoxphos/cn

E1	1	FLUOXIMESTERONE/CN
E2	1	FLUOXIN/CN
E3	0 -->	FLUOXPHOS/CN
E4	1	FLUOXYDIN/CN
E5	1	FLUOXYDINE/CN
E6	1	FLUOXYMESTERONE/CN
E7	1	FLUOXYMESTERONE 3-(O-(CARBOXYMETHOXIME))/CN
E8	1	FLUOXYMESTERONE BIS(TRIMETHYLSILYL) ETHER/CN
E9	1	FLUOXYMESTERONE ENOL TRIS(TRIMETHYLSILYL) ETHER/CN
E10	1	FLUOXYPHENONIUM BROMIDE/CN
E11	1	FLUOXPREDNISOLONE/CN
E12	1	FLUOZIM G 3KH/CN

=> e fluxphos/cn

E1	1	FLUXOMAX CRNIMO 22-1/CN
E2	1	FLUXOTAL/CN
E3	0 -->	FLUXPHOS/CN
E4	1	FLUXREK 01/CN
E5	1	FLUXUM/CN
E6	1	FLUZAMIDE/CN
E7	1	FLUZINAMIDE/CN
E8	2	FLUZON/CN
E9	1	FLUZOPERINE/CN
E10	1	FLVR VAN ART 143.1/CN
E11	1	FLX 113/CN
E12	1	FLX 150/CN

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> e "4,4,4-trifluoro-3-oxobutanoate"/cn

E1	1	4,4,4-TRIFLUORO-3-OXOBUTANAL/CN
E2	1	4,4,4-TRIFLUORO-3-OXOBUTANENITRILE/CN
E3	0 -->	4,4,4-TRIFLUORO-3-OXOBUTANOATE/CN
E4	1	4,4,4-TRIFLUORO-3-OXOBUTANOIC ACID ETHYL ESTER/CN
E5	1	4,4,4-TRIFLUORO-3-OXOBUTANOIC ACID N-(1-METHYL-2-PHENYL-1H-INDOL-5-YL)AMIDE/CN
E6	1	4,4,4-TRIFLUORO-3-OXOBUTANOIC ACID N-(2-PHENYL-1H-INDOL-5-YL)AMIDE/CN
E7	1	4,4,4-TRIFLUORO-3-OXOBUTYRIC ACID/CN
E8	1	4,4,4-TRIFLUORO-3-OXOBUTYRONITRILE/CN
E9	1	4,4,4-TRIFLUORO-3-PHENYL-1,2-BUTADIENE/CN
E10	1	4,4,4-TRIFLUORO-3-PHENYL-2-BUTENOIC ACID ETHYL ESTER/CN
E11	1	4,4,4-TRIFLUORO-3-TRIFLUOROMETHYLBUT-2-ENOIC ACID/CN
E12	1	4,4,4-TRIFLUORO-3-TRIFLUOROMETHYLBUTYRIC ACID/CN

=> d e4

NO L# DEFINED

=> s e4

L1 1 "4,4,4-TRIFLUORO-3-OXOBUTANOIC ACID ETHYL ESTER"/CN

=> d l1

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN

RN 372-31-6 REGISTRY

ED Entered STN: 16 Nov 1984

CN Butanoic acid, 4,4,4-trifluoro-3-oxo-, ethyl ester (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Acetoacetic acid, 4,4,4-trifluoro-, ethyl ester (6CI, 8CI)

OTHER NAMES:

CN 1-Ethoxy-4,4,4-trifluorobutane-1,3-dione
 CN 4,4,4-Trifluoro-3-oxo-butyric acid ethyl ester
 CN 4,4,4-Trifluoro-3-oxobutanoic acid ethyl ester
 CN 4,4,4-Trifluoroacetoacetic acid ethyl ester
 CN Ethyl (trifluoroacetyl)acetate
 CN Ethyl γ,γ,γ -trifluoroacetoacetate
 CN Ethyl ω,ω,ω -trifluoroacetoacetate
 CN Ethyl 3-oxo-4,4,4-trifluorobutanoate
 CN Ethyl 4,4,4-trifluoro-3-oxobutanoate
 CN Ethyl 4,4,4-trifluoro-3-oxobutyrate
 CN Ethyl 4,4,4-trifluoroacetoacetate
 CN Ethyl 4,4,4-trifluoroacetylacetonate
 CN Ethyl trifluoroacetoacetate
 CN NSC 42739
 CN NSC 49750
 MF C6 H7 F3 O3
 CI COM
 LC STN Files: AGRICOLA, BEILSTEIN*, BIOSIS, CA, CAPLUS, CASREACT, CBNB,
 CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, GMELIN*, IFICDB, IFIPAT,
 IFIUDB, PS, SPECINFO, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL, USPATOLD
 (*File contains numerically searchable property data)
 Other Sources: EINECS**, NDSL**, TSCA**
 (**Enter CHEMLIST File for up-to-date regulatory information)

/ Structure 1 in file .gra /

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

783 REFERENCES IN FILE CA (1907 TO DATE)
 9 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 785 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> e "4-chloro-3-oxobutanoate"/cn

E1	1	4-CHLORO-3-OXO-BUTYRIC ACID METHYL ESTER/CN
E2	1	4-CHLORO-3-OXOBUTANANILIDE/CN
E3	0 -->	4-CHLORO-3-OXOBUTANOATE/CN
E4	1	4-CHLORO-3-OXOBUTANOIC ACID/CN
E5	1	4-CHLORO-3-OXOBUTANOIC ACID ETHYL ESTER/CN
E6	1	4-CHLORO-3-OXOBUTANOIC ACID METHYL ESTER/CN
E7	1	4-CHLORO-3-OXOBUTANOYL CHLORIDE/CN
E8	1	4-CHLORO-3-OXOBUTYRIC ACID/CN
E9	1	4-CHLORO-3-OXOBUTYRIC ACID ETHYL ESTER/CN
E10	1	4-CHLORO-3-OXOBUTYRYL CHLORIDE/CN
E11	1	4-CHLORO-3-OXOCARDA-4,14,20(22)-TRIENOLIDE/CN
E12	1	4-CHLORO-3-PENTADECYLPHENOL/CN

=> s e5

L2 1 "4-CHLORO-3-OXOBUTANOIC ACID ETHYL ESTER"/CN

=> d 12

L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
 RN 638-07-3 REGISTRY
 ED Entered STN: 16 Nov 1984
 CN Butanoic acid, 4-chloro-3-oxo-, ethyl ester (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Acetoacetic acid, 4-chloro-, ethyl ester (7CI, 8CI)

OTHER NAMES:

CN γ -Chloroacetoacetic acid ethyl ester
 CN 4-Chloro acetoethylacetate
 CN 4-Chloro-3-oxobutanoic acid ethyl ester
 CN 4-Chloro-3-oxobutyric acid ethyl ester
 CN 4-Chloroacetoacetic acid ethyl ester
 CN Ethyl (chloroacetyl)acetate
 CN Ethyl γ -chloroacetoacetate
 CN Ethyl ω -chloroacetoacetate
 CN Ethyl 3-oxo-4-chlorobutanoate
 CN Ethyl 4-chloro-3-oxobutanoate
 CN Ethyl 4-chloro-3-oxobutyrate
 CN Ethyl 4-chloroacetoacetate
 MF C6 H9 Cl O3
 CI COM
 LC STN Files: AGRICOLA, BEILSTEIN*, BIOSIS, CA, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, IFICDB, IFIPAT, IFIUDB, MEDLINE, MSDS-OHS, PS, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL, USPATOLD
 (*File contains numerically searchable property data)
 Other Sources: DSL**, EINECS**, TSCA**
 (**Enter CHEMLIST File for up-to-date regulatory information)

/ Structure 2 in file .gra /

<http://www.cas.org/legal/infopolicy.html>

=> s l2 near l1
 MISSING OPERATOR L2 NEAR
 The search profile that was entered contains terms or nested terms that are not separated by a logical operator.

=> s l2 and l1
 1035 L2
 785 L1
 L3 40 L2 AND L1

 => s l3 and hydrogenation
 183968 HYDROGENATION
 2474 HYDROGENATIONS
 184230 HYDROGENATION
 (HYDROGENATION OR HYDROGENATIONS)
 L4 8 L3 AND HYDROGENATION

=> d l4 ibib abs 1-8

L4 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2007:362416 CAPLUS <<LOGINID::20081224>>
 DOCUMENT NUMBER: 148:121227
 TITLE: Ruthenium catalyzed asymmetric hydrogenation of α - and β -ketoesters in room temperature ionic liquids using chiral P-Phos ligand
 AUTHOR(S): Xu, Lijin; Lam, Kim Hung; Ruan, Jiwu; Fan, Qinghua; Chan, Albert S. C.
 CORPORATE SOURCE: Open Laboratory of Chirrotechnology of the Institute of Molecular Technology for Drug Discovery and Synthesis and Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, Hong

SOURCE: Kong, Peop. Rep. China
ACS Symposium Series (2007), 950(Ionic Liquids in
Organic Synthesis), 224-234
CODEN: ACSMC8; ISSN: 0097-6156
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 148:121227
AB Chiral dipyridyl phosphine ligand was found to be effective in the
Ru-catalyzed asym. hydrogenation of α - and β -keto
esters in room temperature ionic liqs. with high conversions and good to
excellent enantioselectivities.
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:37762 CAPLUS <<LOGINID::20081224>>
DOCUMENT NUMBER: 144:273900
TITLE: Multigram-scale asymmetric hydrogenation
reactions using Ru-SYNPHOS and Ru-DIFLUORPHOS
catalysts
AUTHOR(S): Jeulin, Severine; Champion, Nicolas; Dellis, Philippe;
Ratovelomanana-Vidal, Virginie; Genet, Jean-Pierre
CORPORATE SOURCE: Laboratoire de Synthese Selective Organique et
Produits Naturels (UMR 7573 CNRS), Ecole Nationale
Superieure de Chimie de Paris, Paris, 75231/05, Fr.
SOURCE: Synthesis (2005), (20), 3666-3671
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:273900
AB The detailed procedure for the synthesis of Ru-SYNPHOS and Ru-DIFLUORPHOS
catalysts are described. These catalysts displayed high rates and are
quite effective for the large-scale hydrogenation reactions of
carbonyl compds., such as β -keto esters RCOCH₂CO₂Et (R = Me, ClCH₂,
F₃C, Ph, PhCH₂OCH₂), acetylacetone and hydroxyacetone.
REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1206596 CAPLUS <<LOGINID::20081224>>
DOCUMENT NUMBER: 144:107747
TITLE: Ruthenium catalyzed asymmetric hydrogenation
of α - and β -keto esters in ionic liquids
using chiral P-Phos ligand
AUTHOR(S): Lam, Kim Hung; Xu, Lijin; Feng, Lichun; Ruan, Jiwu;
Fan, Qinghua; Chan, Albert S. C.
CORPORATE SOURCE: Open Laboratory of Chirotechnology of the Institute of
Molecular Technology for Drug Discovery and Synthesis
and Department of Applied Biology and Chemical
Technology, The Hong Kong Polytechnic University, Hong
Kong, Peop. Rep. China
SOURCE: Canadian Journal of Chemistry (2005), 83(6-7), 903-908
CODEN: CJCHAG; ISSN: 0008-4042
PUBLISHER: National Research Council of Canada
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:107747
AB Chiral dipyridylphosphine ligand was used in the Ru-catalyzed asym.
hydrogenation of α - and β -keto esters in room temperature

ionic liqs. giving the corresponding α - and β -hydroxy esters with high conversions and good to excellent enantioselectivities. The catalyst was recycled by simple extraction and reused five times without loss of activity and enantioselectivity.

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:626146 CAPLUS <<LOGINID::20081224>>

DOCUMENT NUMBER: 141:313992

TITLE: New developments in the synthesis of heterotopic atropisomeric diphosphines via diastereoselective aryl coupling reactions

AUTHOR(S): Madec, Jonathan; Michaud, Guillaume; Genet, Jean-Pierre; Marinetti, Angela

CORPORATE SOURCE: Laboratoire de Synthèse Selective Organique et Produits Naturels, UMR 7573, ENSCP 11, Paris, 75231, Fr.

SOURCE: Tetrahedron: Asymmetry (2004), 15(14), 2253-2261
CODEN: TASYE3; ISSN: 0957-4166

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:313992

AB The new heterotopic atropisomeric diphosphine (R)-5,6-benzo-2,2'-bis(diphenylphosphino)-4',5',6'-trimethylbiphenyl has been prepared. The key step of this synthesis is a diastereoselective, intramol. aryl-aryl coupling reaction via oxidation of a suitable, chiral diarylcuprate. The catalytic properties of the diphosphine in ruthenium promoted hydrogenations of model substrates and in rhodium promoted 1,4-addns. of boronic acids to α,β -unsatd. ketones are fully comparable to those of reference ligands such as BINAP. This seems to indicate that C2-symmetry is not a structural prerequisite for atropisomeric chiral diphosphines to obtain high enantioselectivities in 1,4-addition reactions as well as in hydrogenation reactions.

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:356392 CAPLUS <<LOGINID::20081224>>

DOCUMENT NUMBER: 141:71622

TITLE: Chiral biphenyl diphosphines for asymmetric catalysis: stereoelectronic design and industrial perspectives

AUTHOR(S): Jeulin, Severine; De Paule, Sebastien Duprat; Ratovelomanana-Vidal, Virginie; Genet, Jean-Pierre; Champion, Nicolas; Dellis, Philippe

CORPORATE SOURCE: Laboratoire de Synthèse Selective Organique et Produits Naturels, Ecole Nationale Supérieure de Chimie de Paris, Paris, 75231, Fr.

SOURCE: Proceedings of the National Academy of Sciences of the United States of America (2004), 101(16), 5799-5804
CODEN: PNASA6; ISSN: 0027-8424

PUBLISHER: National Academy of Sciences

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:71622

GI

/ Structure 3 in file .gra /

AB Both enantiomers of the chiral diphosphines I (SYNPHOS) and II (DIFLUORPHOS) are prepared on multigram scales; the electronic and steric characteristics of I and II and of rhodium complexes derived from them are determined, compared with previous diphosphine catalysts, and correlated with their activities and enantioselectivities in the hydrogenation of ketones and olefins. I and II are prepared in five steps from 6-bromo-2,3-dihydro-1,4-benzodioxane and 5-bromo-2,2-difluorobenzodioxole, resp.; lithium-metal exchange and addition to a phosphoryl or phosphinyl chloride followed by oxidation to yield phosphine oxides, regioselective lithiation and iodination, Ullman coupling of the aryl iodides, resolution (either by acid-base resolution with di-O-benzoyl-tartaric acid or by chiral HPLC), and reduction of the phosphine oxides yields I and II in 38% and 33% overall yield, resp. The bite angles of I and II are compared to those of other common diphosphine ligands such as BINAP and MeO-BIPHEP. The structure of diastereomeric chlorohydridoruthenium complexes of (S)-II with Me acetoacetate is determined. The C-O stretching frequencies of chloro(carbonyl)rhodium diphosphine complexes containing I, II, BINAP, and MeO-BIPHEP are determined as a measure of the electronic demands of the diphosphine ligands. β -Keto ester, α -keto ester, 1,3-diketone, ketone, and olefin substrates are hydrogenated in the presence of nonracemic I, II, BINAP, and MeO-BIPHEP and bis(η 3-methylallyl)(η 4-1,5-cyclooctadienyl)ruthenium; the enantioselectivities are correlated with the steric and electronic properties of the ligands. The stereoelectronic features of the ligand and the substrate deeply influence the enantioselectivities obtained in asym. hydrogenation; whereas the steric and electronic factors for I (as in other diphosphines) correlate well, the bite angle of II does not correlate to its electronic effects in asym. hydrogenation reactions, leading to complementary hydrogenation selectivities for ligands I and II.

REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2004:70307 CAPLUS <<LOGINID::20081224>>
 DOCUMENT NUMBER: 140:253116
 TITLE: Difluorophos, an electron-poor diphosphane: A good match between electronic and steric features
 AUTHOR(S): Jeulin, Severine; Duprat de Paule, Sebastien; Ratovelomanana-Vidal, Virginie; Genet, Jean-Pierre; Champion, Nicolas; Dellis, Philippe
 CORPORATE SOURCE: Laboratoire de Synthese Selective Organique et Produits Naturels, Ecole Nationale Supérieure de Chimie de Paris, Paris, 75231, Fr.
 SOURCE: Angewandte Chemie, International Edition (2004), 43(3), 320-325
 CODEN: ACIEF5; ISSN: 1433-7851
 PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 140:253116
 GI

/ Structure 4 in file .gra /

AB Both enantiomers of difluorophos I were synthesized and their

stereoelectronic features were evaluated in theor. and exptl. studies. The unusual π acidity of I explains the excellent results obtained with it in ruthenium-mediated asym. hydrogenation of fluorinated β -functionalized ketones. These results are better than those obtained with other biphenyl-based diphosphines.

REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:502611 CAPLUS <<LOGINID::20081224>>

DOCUMENT NUMBER: 121:102611

ORIGINAL REFERENCE NO.: 121:18339a,18342a

TITLE: purification and characterization of a novel carbonyl reductase isolated from *Rhodococcus erythropolis*

AUTHOR(S): Zelinski, Thomas; Peters, Joerg; Kula, Maria-Regina

CORPORATE SOURCE: Institut fuer Enzymtechnologie der Heinrich-Heine-Universitaet Duesseldorf, Forschungszentrum Juelich (KFA), Julich, 52404, Germany

SOURCE: Journal of Biotechnology (1994), 33(3), 283-92
CODEN: JBITD4; ISSN: 0168-1656

DOCUMENT TYPE: Journal

LANGUAGE: English

AB During growth on n-tetradecane a novel NADH-dependent carbonyl reductase is induced in the Gram-pos. bacterium *Rhodococcus erythropolis* (Peters, P., Zelinski, T. and Kula, M.R. (1992) Appl. microbiol. biotechnol. 38, 334-340). The enzyme has been purified to homogeneity using fractional pH precipitation, anion exchange chromatog. and affinity chromatog. The isoelec. point of the oxidoreductase is 4.4. The apparent mol. mass of the native enzyme is 161 kDa, that of the subunits 40 kDa as determined by SDS gel electrophoresis. A tetrameric structure of the carbonyl reductase is consistent with these results. Important biochem. data concerning the application of the reductase are: a broad pH-optimum, temperature optimum at 40° and stability at room temperature for more than 5 days. The oxidoreductase accepted as substrate aliphatic and aromatic ketones, keto esters

(esters of keto carboxylic acids) and halogenated carbonyl compds. and reduced them to the corresponding hydroxyl compds. with (S)-configuration with more than 98% enantiomeric excess. The NAD⁺-dependent oxidation of primary alcs. was not catalyzed by the carbonyl reductase, whereas secondary alcs. and hydroxy acid esters were oxidized to the corresponding carbonyl compds. at about 10-fold slower reaction rates compared to the reduction

L4 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1993:603787 CAPLUS <<LOGINID::20081224>>

DOCUMENT NUMBER: 119:203787

ORIGINAL REFERENCE NO.: 119:36369a,36372a

TITLE: Stereodivergent synthesis of fluorinated threonine derivatives in high optical purity

AUTHOR(S): Shimizu, Makoto; Yokota, Tetsuya; Fujimori, Kouichi; Fujisawa, Tamotsu

CORPORATE SOURCE: Dep. Chem. Mater., Mie Univ., Tsu, 514, Japan

SOURCE: Tetrahedron: Asymmetry (1993), 4(5), 835-8
CODEN: TASYE3; ISSN: 0957-4166

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 119:203787

AB Fluorinated 3-acetoxy-2-(methoxyimino)butyrates were resolved by lipase to give the corresponding alcs. and the acetates in high optical purity. The resolved alcs. were readily converted into mono-, di-, and

trifluorothreonine and allothreonine derivs. by hydrogenation of
the methoxyimino group.

<http://www.cas.org/legal/infopolicy.html>

=> SAVE L4 SA577385/A

ANSWER SET L4 HAS BEEN SAVED AS 'SA577385/A'

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> e "4,4,4-trichloro-3-hydroxybutarate"/cn

E1	1	4,4,4-TRICHLORO-2-METHYLBUTYRONITRILE/CN
E2	1	4,4,4-TRICHLORO-2-METHYLCROTONALDEHYDE/CN
E3	0 -->	4,4,4-TRICHLORO-3-HYDROXYBUTARATE/CN
E4	1	4,4,4-TRICHLORO-3-HYDROXYBUTYRIC ACID/CN
E5	1	4,4,4-TRICHLORO-3-HYDROXYBUTYRONITRILE/CN
E6	1	4,4,4-TRICHLORO-3-METHYLBUTANENITRILE/CN
E7	1	4,4,4-TRICHLORO-3-METHYLBUTYRONITRILE/CN
E8	1	4,4,4-TRICHLORO-N-(3-(3-(THIEN-2-YL)CARBONYL)PYRAZOLO(1,5-A)PYRIMIDIN-7-YL)PHENYL)BUTANAMIDE/CN
E9	1	4,4,4-TRICHLOROACETOACETYL CHLORIDE/CN
E10	1	4,4,4-TRICHLOROBUTAN-1-OL/CN
E11	1	4,4,4-TRICHLOROBUTANENITRILE/CN
E12	1	4,4,4-TRICHLOROBUTYL ACETATE/CN

=> e "ethyl 4,4,4-trichloro-3-hydroxybutarate"/cn

E1	1	ETHYL 4,4,4-TRICHLORO-2-CYANOCROTONATE/CN
E2	1	ETHYL 4,4,4-TRICHLORO-3-HYDROXYBUTANOATE/CN
E3	0 -->	ETHYL 4,4,4-TRICHLORO-3-HYDROXYBUTARATE/CN
E4	1	ETHYL 4,4,4-TRICHLORO-3-OXOBUTANOATE/CN
E5	1	ETHYL 4,4,4-TRICHLOROACETOACETATE/CN
E6	1	ETHYL 4,4,4-TRICHLOROBUTANOATE/CN
E7	1	ETHYL 4,4,4-TRICHLOROBUTENOATE/CN
E8	1	ETHYL 4,4,4-TRICHLOROBUTYRATE/CN
E9	1	ETHYL 4,4,4-TRIFLUORO-2-((2-HYDROXYETHYL)THIO)-3-OXOBUTANOAT E/CN
E10	1	ETHYL 4,4,4-TRIFLUORO-2-BUTENOATE/CN
E11	1	ETHYL 4,4,4-TRIFLUORO-2-BUTYNECARBOXYLATE/CN
E12	1	ETHYL 4,4,4-TRIFLUORO-2-BUTYNOATE/CN

=> s e2

L1 1 "ETHYL 4,4,4-TRICHLORO-3-HYDROXYBUTANOATE"/CN

=> d l1

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
RN 19486-93-2 REGISTRY
ED Entered STN: 16 Nov 1984
CN Butanoic acid, 4,4,4-trichloro-3-hydroxy-, ethyl ester (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Butyric acid, 4,4,4-trichloro-3-hydroxy-, ethyl ester (6CI, 7CI, 8CI)
OTHER NAMES:
CN Ethyl 4,4,4-trichloro-3-hydroxybutanoate
MF C6 H9 Cl3 O3
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS, TOXCENTER,
USPAT2, USPATFULL
(*File contains numerically searchable property data)

/ Structure 5 in file .gra /

<http://www.cas.org/legal/infopolicy.html>

=> s 11 and hydrogenation

18 L1
183968 HYDROGENATION
2474 HYDROGENATIONS
184230 HYDROGENATION
(HYDROGENATION OR HYDROGENATIONS)

L2 1 L1 AND HYDROGENATION

=> d 12

L2 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2005:393998 CAPLUS <<LOGINID::20081224>>

DN 142:429938

TI Stereoselective catalytic hydrogenation process for the
preparation of (S)- or (R)-4-halo-3-hydroxybutyrate esters from the
corresponding 4-halo-3-oxobutyrate

PA Lonza AG, Switz.

SO Eur. Pat. Appl., 9 pp.

CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	---	-----	-----	-----
PI	EP 1528053	A1	20050504	EP 2003-24865	20031031
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	AU 2004291249	A1	20050602	AU 2004-291249	20041022
	CA 2541716	A1	20050602	CA 2004-2541716	20041022
	WO 2005049545	A1	20050602	WO 2004-EP11971	20041022
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, VZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	EP 1682481	A1	20060726	EP 2004-790763	20041022
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
	CN 1874989	A	20061206	CN 2004-80032075	20041022
	BR 2004016133	A	20070102	BR 2004-16133	20041022
	JP 2007509874	T	20070419	JP 2006-537143	20041022
	KR 2006095769	A	20060901	KR 2006-708041	20060426
	NO 2006002131	A	20060530	NO 2006-2131	20060512
	IN 2006DN03081	A	20070810	IN 2006-DN3081	20060529
	US 20070078279	A1	20070405	US 2006-577385	20060703
PRAI	EP 2003-24865	A	20031031		
	WO 2004-EP11971	W	20041022		

OS CASREACT 142:429938; MARPAT 142:429938

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> d l1 ibib abs all
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:y
L1  ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2008 ACS on STN
RN  19486-93-2  REGISTRY
ED  Entered STN:  16 Nov 1984
CN  Butanoic acid, 4,4,4-trichloro-3-hydroxy-, ethyl ester  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN  Butyric acid, 4,4,4-trichloro-3-hydroxy-, ethyl ester (6CI, 7CI, 8CI)
OTHER NAMES:
CN  Ethyl 4,4,4-trichloro-3-hydroxybutanoate
MF  C6 H9 Cl3 O3
LC  STN Files:  BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS, TOXCENTER,
      USPAT2, USPATFULL
      (*File contains numerically searchable property data)
DT.CA  Caplus document type:  Journal; Patent
RL.P  Roles from patents:  PREP (Preparation); USES (Uses)
RL.NP  Roles from non-patents:  PREP (Preparation); PRP (Properties); RACT
      (Reactant or reagent); NORL (No role in record)
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/ Structure 6 in file .gra /
REFERENCE 1
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AN  142:429938  CA <<LOGINID::20081224>>
TI  Stereoselective catalytic hydrogenation process for the preparation of
    (S)- or (R)-4-halo-3-hydroxybutyrate esters from the corresponding
    4-halo-3-oxobutyrate
PA  Lonza AG, Switz.
SO  Eur. Pat. Appl., 9 pp.
    CODEN: EPXXDW
DT  Patent
LA  English
IC  ICM  C07C067-31
    ICS  C07C069-675
CC  23-17 (Aliphatic Compounds)
    Section cross-reference(s): 67
```

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1528053	A1	20050504	EP 2003-24865	20031031
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
AU 2004291249	A1	20050602	AU 2004-291249	20041022
CA 2541716	A1	20050602	CA 2004-2541716	20041022
WO 2005049545	A1	20050602	WO 2004-EP11971	20041022
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1682481	A1	20060726	EP 2004-790763	20041022
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
CN 1874989	A	20061206	CN 2004-80032075	20041022
BR 2004016133	A	20070102	BR 2004-16133	20041022

	JP	2007509874	T	20070419	JP	2006-537143	20041022
	KR	2006095769	A	20060901	KR	2006-708041	20060426
	NO	2006002131	A	20060530	NO	2006-2131	20060512
	IN	2006DN03081	A	20070810	IN	2006-DN3081	20060529
	US	20070078279	A1	20070405	US	2006-577385	20060703
PRAI	EP	2003-24865		20031031			
GI	WO	2004-EP11971		20041022			

/ Structure 7 in file .gra /

AB Enantiomerically pure (S)- or (R)-4-halo-3-hydroxybutyrates [I; II; R1 = CH2X, CHX2, CX3; X = Cl and/or Br; R2 = C1-6 alkyl, C3-8 cycloalkyl, (un)substituted aryl, (un)substituted aralkyl; e.g., Et (3S)-4-chloro-3-hydroxybutyrate] are prepared in high yield and selectivity by the asym. hydrogenation of 4-halo-3-oxobutyrate esters R1C(:O)CH2CO2R2 (e.g., Et 4-chloro-3-oxobutyrate) in the presence of a catalyst of a ruthenium complex comprising a chiral diphosphine ligand (III).

ST chiral halohydroxybutyrate ester prepn stereoselective catalytic hydrogenation halo-oxobutyrate; asym ethyl chlorohydroxybutyrate prepn stereoselective catalytic hydrogenation chlorooxobutyrate

IT Alcohols, uses
 RL: NUU (Other use, unclassified); USES (Uses)
 (C1-4, solvents; stereoselective catalytic hydrogenation process for the preparation of (S)- or (R)-4-halo-3-hydroxybutyrate esters from the corresponding 4-halo-3-oxobutyrate using)

IT Carboxylic acids, preparation
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (esters, chiral 4-halo-3-hydroxybutyrates; stereoselective catalytic hydrogenation process for the preparation of (S)- or (R)-4-halo-3-hydroxybutyrate esters from the corresponding 4-halo-3-oxobutyrate)

IT Stereochemistry
 (stereoselective catalytic hydrogenation process for the preparation of (S)- or (R)-4-halo-3-hydroxybutyrate esters from the corresponding 4-halo-3-oxobutyrate)

IT Hydrogenation catalysts
 (stereoselective, ruthenium complex comprising a chiral diphosphine ligand; stereoselective catalytic hydrogenation process for the preparation of (S)- or (R)-4-halo-3-hydroxybutyrate esters from the corresponding 4-halo-3-oxobutyrate)

IT Hydrogenation
 (stereoselective; stereoselective catalytic hydrogenation process for the preparation of (S)- or (R)-4-halo-3-hydroxybutyrate esters from the corresponding 4-halo-3-oxobutyrate)

IT 10049-08-8, Ruthenium trichloride 52462-29-0 503538-69-0 503538-70-3
 RL: CAT (Catalyst use); USES (Uses)
 (in a stereoselective catalytic hydrogenation process for the preparation of (S)- or (R)-4-halo-3-hydroxybutyrate esters from the corresponding 4-halo-3-oxobutyrate)

IT 1333-74-0, Hydrogen, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (in a stereoselective catalytic hydrogenation process for the preparation of (S)- or (R)-4-halo-3-hydroxybutyrate esters from the corresponding 4-halo-3-oxobutyrate)

IT 67-68-5, DmsO, uses 68-12-2, Dmf, uses 75-05-8, Acetonitrile, uses
 RL: NUU (Other use, unclassified); USES (Uses)

(solvent; stereoselective catalytic hydrogenation process for the preparation of (S)- or (R)-4-halo-3-hydroxybutyrate esters from the corresponding 4-halo-3-oxobutyrate using)

IT 638-07-3, Ethyl 4-chloro-3-oxobutyrate
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (stereoselective catalytic hydrogenation process for the preparation of (S)- or (R)-4-halo-3-hydroxybutyrate esters from the corresponding 4-halo-3-oxobutyrate)

IT 19486-93-2P 86728-85-0P 90866-33-4P 125537-59-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (stereoselective catalytic hydrogenation process for the preparation of (S)- or (R)-4-halo-3-hydroxybutyrate esters from the corresponding 4-halo-3-oxobutyrate)

IT 3702-98-5 74530-56-6, tert-Butyl 4-chloro-3-oxobutyrate
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (stereoselective catalytic hydrogenation process for the preparation of (S)- or (R)-4-halo-3-hydroxybutyrate esters from the corresponding 4-halo-3-oxobutyrate using)

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD

- (1) Duprat de Paule Sebastien; WO 03029259 A 2003
- (2) Pai, C; TETRAHEDRON LETTERS 2002, V43(15), P2789 CAPLUS
- (3) Takasago Perfumery Co Ltd; EP 0295109 A 1988 CAPLUS
- (4) Takasago Perfumery Co Ltd; EP 0339764 A 1989 CAPLUS
- (5) Takasago Perfumery Co Ltd; EP 1176135 A 2002 CAPLUS

REFERENCE 2

AN 137:369737 CA <<LOGINID::20081224>>

TI Stereoselective hydrogen-transfer process and chiral ruthenium-diamine complex catalyst for producing optically active β -hydroxycarboxylate esters from β -ketocarboxylate esters and hydrogen donors

IN Tada, Kenichi; Miura, Takashi

PA Takasago International Corporation, Japan

SO Eur. Pat. Appl., 9 pp.
 CODEN: EPXXDW

DT Patent

LA English

IC ICM C07C067-317

CC 23-17 (Aliphatic Compounds)
 Section cross-reference(s): 67

FAN.CNT 13

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1258470	A2	20021120	EP 2002-291172	20020510
	EP 1258470	A3	20030813		
	EP 1258470	B1	20050817		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2003034665	A	20030207	JP 2002-82865	20020325
	JP 4015450	B2	20071128		
	ES 2247280	T3	20060301	ES 2002-291172	20020510
	US 20030004362	A1	20030102	US 2002-142983	20020513
	US 6723871	B2	20040420		
PRAI	JP 2001-150012		20010518		
	JP 2002-82865		20020325		

GI

/ Structure 8 in file .gra /

AB Optically active β -hydroxycarboxylate esters $R_1CH(OH)CH_2CO_2R_2$ [$R_1 =$

C1-10 (un)branched perfluoroalkyl or perchloroalkyl; R2 = C1-8 lower alkyl, (un)substituted benzyl; e.g., optically active Et 4,4,4-trifluoro-3-hydroxybutanoate] are prepared in high yield and selectivity by stereoselective hydrogen transfer to the corresponding β -ketocarboxylate esters R1COCH2CO2R2 (e.g., Et 4,4,4-trifluoro-3-oxobutanoate) in the presence of hydrogen donors (e.g., formic acid-triethylamine mixts.) and a chiral ruthenium-diamine complex catalyst [I; * = asym. carbon atom; R3, R4 = alkyl, Ph, (un)substituted cycloalkyl; R5 = methanesulfonyl, trifluoromethanesulfonyl, benzenesulfonyl, (un)substituted naphthyl, camphorsulfonyl, alkoxy carbonyl, (un)substituted benzoyl; R6 = H, alkyl; A = (un)substituted aromatic compound; X = halogen; e.g., RuCl[(1R,2R)-p-TsNHCH(C6H5)CH(C6H5)NH2] (p-cymene)].

ST stereoselective hydrogen transfer optically active hydroxycarboxylate ester prepn; chiral ruthenium diamine complex catalyst stereoselective hydrogen transfer; optically active ethyl trifluorohydroxybutanoate prepn stereoselective hydrogen transfer

IT Esters, preparation
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (hydroxy, chiral β -hydroxycarboxylate esters; stereoselective hydrogen-transfer process and chiral ruthenium-diamine complex catalyst for producing optically active β -hydroxycarboxylate esters from β -ketocarboxylate esters and hydrogen donors)

IT Esters, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (keto, β -ketocarboxylate esters; stereoselective hydrogen-transfer process and chiral ruthenium-diamine complex catalyst for producing optically active β -hydroxycarboxylate esters from β -ketocarboxylate esters and hydrogen donors)

IT Stereochemistry
 (stereoselective hydrogen-transfer process and chiral ruthenium-diamine complex catalyst for producing optically active β -hydroxycarboxylate esters from β -ketocarboxylate esters and hydrogen donors)

IT Hydrogen transfer catalysts
 (stereoselective, chiral ruthenium-diamine complex; chiral ruthenium-diamine complex catalyst for producing optically active β -hydroxycarboxylate esters from β -ketocarboxylate esters and hydrogen donors)

IT Hydrogen transfer
 (stereoselective; stereoselective hydrogen-transfer process and chiral ruthenium-diamine complex for producing optically active β -hydroxycarboxylate esters from β -ketocarboxylate esters and hydrogen donors)

IT 192139-92-7
 RL: CAT (Catalyst use); USES (Uses)
 (stereoselective hydrogen-transfer process and chiral ruthenium-diamine complex catalyst for producing optically active β -hydroxycarboxylate esters from β -ketocarboxylate esters and hydrogen donors)

IT 372-31-6, Ethyl 4,4,4-trifluoro-3-oxobutanoate 3702-98-5, Ethyl 4,4,4-trichloro-3-oxobutanoate 83643-84-9, Methyl 4,4,4-trifluoro-3-oxobutanoate 175230-50-9, Isopropyl 4,4,4-trifluoro-3-oxobutanoate 475467-54-0, Methyl 3-oxo-4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-pentadecafluorodecanoate
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (stereoselective hydrogen-transfer process and chiral ruthenium-diamine complex catalyst for producing optically active β -hydroxycarboxylate esters from β -ketocarboxylate esters and hydrogen donors)

IT 64-18-6, Formic acid, reactions 75-50-3, Trimethylamine, reactions

RL: RCT (Reactant); RGT (Reagent); RACT (Reactant or reagent)
(stereoselective hydrogen-transfer process and chiral ruthenium-diamine
complex catalyst for producing optically active
 β -hydroxycarboxylate esters from β -ketocarboxylate esters and
hydrogen donors)

IT 372-30-5P, Ethyl 4,4,4-trifluoro-3-hydroxybutanoate 19486-93-2P, Ethyl
4,4,4-trichloro-3-hydroxybutanoate 305322-80-9P, Isopropyl
4,4,4-trifluoro-3-hydroxybutanoate 475467-53-9P, Methyl
4,4,4-trifluoro-3-hydroxybutanoate 475467-55-1P, Methyl
3-hydroxy-4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-pentadecafluorodecanoate

RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective hydrogen-transfer process and chiral ruthenium-diamine
complex catalyst for producing optically active
 β -hydroxycarboxylate esters from β -ketocarboxylate esters and
hydrogen donors)

REFERENCE 3

AN 100:22738 CA <<LOGINID::20081224>>
TI Heterosubstituted (silicon, germanium) 2-oxetanones. Reaction of silyl-
and germylketenes with polyfluorinated ketones and properties of
3-silyl(germyl)-2-oxetanones

AU Zaitseva, G. S.; Livantsova, L. I.; Bekker, R. A.; Baukov, Yu. I.;
Lutsenko, I. F.

CS Mosk. Gos. Univ., Moscow, USSR

SO Zhurnal Obshchei Khimii (1983), 53(9), 2068-77

CODEN: ZOKHA4; ISSN: 0044-460X

DT Journal

LA Russian

CC 29-8 (Organometallic and Organometalloidal Compounds)

GI

/ Structure 9 in file .gra /

AB Reaction of silyl- and germylketenes (e.g., Me₃SiCH:CO) with
polyfluorinated ketones [e.g., (CF₃)₃CO] gave a mixture of 1:1 cycloadducts
(2-oxetanones, e.g., I) and 2:1 cyclodimers, e.g., II. Some reactions of
the oxetanones were studied.

ST ketone polyfluoro cycloaddn ketene; silylketene cycloaddn polyfluoro
ketone; germylketene cycloaddn polyfluoro ketone; oxetanone silyl germyl

IT Cycloaddition reaction

(of silyl- and germylketenes with polyfluorinated ketones)

IT 79305-64-9P 83740-52-7P

RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(formation and reaction of, with (trimethylsilyl)ketene)

IT 67354-06-7P 67354-19-2P 67354-21-6P 67354-23-8P 67354-24-9P

67354-25-0P 67354-26-1P 88237-28-9P 88237-29-0P 88237-30-3P

88237-31-4P 88237-32-5P 88237-33-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(preparation and reactions of)

IT 4964-02-7P 4964-03-8P 4964-04-9P 4964-05-0P 13159-46-1P

19486-93-2P 24099-72-7P 56183-55-2P 56183-56-3P 62019-87-8P

67354-12-5P 67354-13-6P 67354-15-8P 67354-16-9P 67354-17-0P

67354-18-1P 75668-12-1P 80673-03-6P 88237-34-7P 88237-35-8P

88237-36-9P 88237-37-0P 88237-38-1P 88237-39-2P 88237-40-5P

88237-41-6P 88237-42-7P 88237-43-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

IT 127-21-9 421-50-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with ketenes)

IT 64-17-5, reactions 109-89-7, reactions 121-44-8, reactions 124-40-3,
 reactions 2083-91-2 7727-15-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with oxetanones)

IT 4071-85-6 32278-84-5
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with polyfluorinated ketones)

REFERENCE 4

AN 96:68256 CA <<LOGINID::20081224>>
 TI New syntheses of trichloromethyl functional alcohols. Studies of their
 tranquilizing properties

AU Deleris, Gerard; Dunogues, Jacques; Babin, Pierre; Calas, Raymond;
 Bardone, Marie Claude; Guyonnet, Jean Claude
 CS Lab. Chim. Org. Composes Org. Silicium Etain, CNRS, Talence, 33405, Fr.
 SO European Journal of Medicinal Chemistry (1981), 16(6), 533-7
 CODEN: EJMCA5; ISSN: 0009-4374

DT Journal
 LA French
 CC 23-7 (Aliphatic Compounds)
 Section cross-reference(s): 1

AB CCl3CHROH (I, R = BuC.tplbond.C, Me3SiC.tplbond.C, Me3SiCH2C.tplbond.C,
 PhC.tplbond.C, 3-pyridylethynyl, EtO2CCH2, Et2NCOCH2, 2-pyridyl) were
 prepared by treating RSiMe3 with chloral, and methanolysis of Cl3CCHROSiMe3.
 I(R = Et2NCOCH2, 2-pyridyl) had tranquilizing activity comparable to that
 of meprobamate, the pyridine derivative being free of convulsant side-effects.

ST trichlorobutynol prepn tranquilizer

IT Tranquilizers and Neuroleptics
 (trichlorobutynols)

IT 57212-16-5P 57212-18-7P 57212-20-1P 80673-03-6P 80673-04-7P
 80673-05-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and desilylation of)

IT 25290-15-7P 57212-17-6P 57212-19-8P 57212-21-2P 80673-02-5P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological
 study, unclassified); SPN (Synthetic preparation); BIOL (Biological
 study); PREP (Preparation)
 (preparation and pharmacol. activity of)

IT 2170-06-1P 3844-94-8P 4071-88-9P 13737-04-7P 14630-40-1P
 21752-80-7P 23138-65-0P 80673-00-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and reaction of, with chloral)

IT 6181-26-6P 19486-93-2P 80673-01-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

IT 75-87-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with trimethylsilylalkynes)

IT 105-39-5 109-04-6 127-18-4, reactions 536-74-3 627-41-8 693-02-7
 1121-55-7 2315-36-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (silylation of)

REFERENCE 5

AN 95:2477 CA <<LOGINID::20081224>>
 TI Latent inhibitors. Part 2. Allylic inhibitors of alcohol dehydrogenase
 AU MacInnes, Iain; Schorstein, David E.; Suckling, Colin J.; Wrigglesworth, Roger
 CS Dep. Pure Appl. Chem., Univ. Strathclyde, Glasgow, G1 1XL, UK
 SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1981), (4), 1103-8
 CODEN: JCPRB4; ISSN: 0300-922X
 DT Journal
 LA English
 CC 7-3 (Enzymes)
 AB Of a number of 3-substituted prop-2-en-1-ols and -1-als tested for latent inhibition of horse liver alc. dehydrogenase (EC 1.1.1.1), only 3-ethylthioprop-2-en-1-ol was active, via oxidation to the corresponding aldehyde catalyzed by the enzyme. Product studies and kinetic detns. indicated that the persistence of inhibition was due to EtSH, formed by an enzyme-catalyzed hydrolysis of the aldehyde. The preparation of the inhibitors is described.
 ST liver alc dehydrogenase propenol propenal
 IT Liver, composition
 (alc. dehydrogenase of, propenols and propenals latent inhibition of)
 IT 107-18-6, biological studies 107-19-7 16263-71-1 37675-33-5
 56772-86-2 67935-24-4 77889-97-5 77889-98-6 77889-99-7
 77890-00-7 77890-97-2 77890-98-3
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
 (alc. dehydrogenase of liver response to)
 IT 623-47-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (bromination of)
 IT 9031-72-5
 RL: PROC (Process)
 (of liver, propenols and propenals latent inhibition of)
 IT 77890-03-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (oxidative deethylation of)
 IT 2579-22-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (phenoxylation of)
 IT 19486-93-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and oxidation of)
 IT 13001-71-3P 42844-38-2P 77890-01-8P 77890-02-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reduction of)
 IT 75-87-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with Et bromoacetate)
 IT 75-08-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with Et propiolate)
 IT 105-36-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with chloral)
 IT 624-67-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with ethanethiol)
 IT 75-89-8 100-02-7, reactions 108-95-2, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with phenylpropynal)
 IT 504-17-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with tetraethoxypropane)
 IT 122-31-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with thiobarbituric acid)
 IT 2579-22-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with trifluoroethanol)

REFERENCE 6

AN 94:22995 CA <<LOGINID::20081224>>
 TI Pressure- or heat-sensitive recording material
 IN Petitpierre, Jean Claude
 PA Ciba-Geigy A.-G., Switz.
 SO Ger. Offen., 30 pp.
 CODEN: GWXXBX
 DT Patent
 LA German
 IC B41M005-12; B41M005-18
 CC 74-8 (Radiation Chemistry, Photochemistry, and Photographic Processes)
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2946830	A1	19800529	DE 1979-2946830	19791120
	DE 2946830	C2	19811029		
	US 4291901	A	19810929	US 1979-95119	19791116
	EP 12112	A1	19800611	EP 1979-810160	19791119
	EP 12112	B1	19831005		
	R: AT, BE, CH, DE, FR, GB, IT				
	FI 7903646	A	19800524	FI 1979-3646	19791121
	CA 1139559	A1	19830118	CA 1979-340288	19791121
	JP 55073586	A	19800603	JP 1979-152367	19791122
	JP 63043236	B	19880829		
	FR 2442139	A1	19800620	FR 1979-28857	19791122
	FR 2442139	B1	19810227		
	BR 7907589	A	19800805	BR 1979-7589	19791122
	GB 2047417	A	19801126	GB 1979-40479	19791122
	GB 2047417	B	19830420		
PRAI	CH 1978-12026		19781123		
	CH 1979-9628		19791026		

AB Pressure- or heat-sensitive recording materials using a system composed of a reactive combination of a color developer and a color former contain a compound of the general formula RCHOHZR1m (R = a reactive organic methylene or Me compound, R2R3N, R1mZ1CHOHNr4NZ2NR2, or R5S where R2, R3, R4 = H, substituted or unsubstituted alkyl, aralkyl, alkanoyl, alkylsulfonyl, aroyl, arylsulfonyl, cyanoamidino, substituted carbamoyl, or substituted sulfamoyl; Z1 = alkylene, arylene, or aralkylene; Z2 = CO, SO2 COCO, substituted carbonylmethylenecarbonyl, alkylene, or phenylene; R5 = substituted or unsubstituted alkyl, aralkyl, aryl, or a 5-membered heterocycle; R1 = halogen, CN, or NO2; Z = same as Z1; m = 1-6) as the color developer. Thus, a mixture containing PhNHCONHCHOHCCl3 32, the distearylamine of ethylenediamine 3.8, kaolin 39, poly(vinyl alc) (88% hydrolyzed) 20 g, and water 500 mL was ball-milled to a particle size of 5 μ . In a 2nd ball mill was milled a mixture of 2-phenylamino-3-methyl-6-diethylaminofluoran 6, poly(vinyl alc.) (88% hydrolyzed) 3, and water 60 mL to give a particle size of .apprx.3 μ . Both dispersion were then combined and cooled at 5.5 g/m2 on a paper support. Application of a heated ball-point pen to the paper gave an

intense black color that had excellent lightfastness.

ST color developer pressure thermal recording; thermal recording color developer; copying pressure sensitive color developer; urea deriv color developer copying

IT Thermography
(heat-sensitive compns. for, containing urea derivs. as color developers)

IT Copying paper
(pressure-sensitive, color developers for, urea derivs. as)

IT 57-13-6D, derivs. 116-52-9 760-40-7 1552-33-6 5445-85-2
6316-07-0 13505-41-4 15446-11-4 19177-72-1 19486-93-2 31339-87-4
33243-78-6 42840-67-5 53376-31-1 54888-09-4 69796-31-2
75456-90-5 75456-91-6 75456-92-7 75456-93-8 75456-94-9
75456-95-0 75456-96-1 75456-97-2 75456-98-3 75456-99-4
75457-00-0 75457-01-1 75457-02-2 75457-03-3 75457-04-4
75457-05-5 75457-06-6 75457-07-7 75457-08-8

RL: USES (Uses)
(color developer, for pressure- or heat-sensitive recording materials)

IT 110-30-5 1552-42-7 29512-49-0
RL: USES (Uses)
(pressure-sensitive copying materials containing urea derivative color developer and)

REFERENCE 7

AN 87:52713 CA <<LOGINID::20081224>>

TI Reaction of chloral with ortho esters and acetaldehyde acetal

AU Petrov, K. A.; Tikhonova, N. A.; Shchekotikhina, N. A.

CS USSR

SO Zhurnal Organicheskoi Khimii (1977), 13(5), 939-43
CODEN: ZORKAE; ISSN: 0514-7492

DT Journal

LA Russian

CC 23-17 (Aliphatic Compounds)

AB Cl3CHO (I) reacted with HC(OEt)3 containing H2SO4, dry HCl or ZnCl2 to give Cl3CCH(OH)OEt (II) and Cl3CCH(OEt)2. Treating II with MeC(OEt)3 in C6H6 containing ZnCl2 at 120° yielded 12.5% Cl3CCH(OH)CH2CO2Et and 56.5% Cl3CCH:CHCO2Et. I reacted with RC(OR1)3 (R = H, R1 = Me, Et; R = EtO, R1 = Et) containing NaOAc to give 50-70% Cl3CCH(OR1)OCR(OR1)2 (III). Alcoholysis of III (R = H, R1 = Me, Et) gave up to quant. yields of Cl3CCH(OH)OR1 and HC(OR1)3. Reacting I with MeCH(OEt)2 gave 25% Cl3CCH(OEt)OCHMeOEt in the absence of catalyst and CH2:CHOEt and II in quant. yield in the presence of anhydrous NaOAc.

ST chloral reaction ortho ester acetal

IT 63504-87-0P 63504-89-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and alcoholysis of)

IT 515-83-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with ethyl orthoformate)

IT 109-92-2P 599-97-3P 2791-89-1P 13001-71-3P 19486-93-2P
63504-88-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 105-57-7 122-51-0 149-73-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chloral)

IT 78-39-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chloral hydrate)

IT 302-17-0

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ethyl orthoacetate)
IT 75-87-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ortho esters and with acetaldehyde diethyl acetal)

REFERENCE 8

AN 75:42672 CA <<LOGINID::20081224>>
TI Spectroscopic study of an intramolecular hydrogen bond in
hydroxycarboxylic acids and their esters
AU Abramovich, M. A.; Ginzburg, I. M.; Ioffe, D. V.
CS Leningr. Khim.-Farm. Inst., Leningrad, USSR
SO Teoreticheskaya i Eksperimental'naya Khimiya (1971), 7(2), 225-31
CODEN: TEKHA4; ISSN: 0497-2627
DT Journal
LA Russian
CC 73 (Spectra by Absorption, Emission, Reflection, or Magnetic Resonance,
and Other Optical Properties)
AB Frequencies of stretching vibrations (ν) of OH and CO groups of 10
hydroxycarboxylic acids and their esters (CCl₄ solns.) were studied with
respect to the formation of intramol. H bonds. Effect of substituents on
the strength of the H bonds and, therefore, on ν is discussed.
ST hydroxy carboxylic acid hydrogen bond; IR hydroxy carboxylic acid
IT Hydrogen bonds
(in hydroxycarboxylic acids, ir spectra in relation to)
IT Spectra, infrared
REFERENCE 9

AN 74:76484 CA <<LOGINID::20081224>>
TI Organotin compounds. XXIII. Reformatsky-type reactions with
 α -functionally substituted organotin compounds
AU Noltes, Jan G.; Verbeek, F.; Creemers, Henricus M. J. C.
CS Inst. Org. Chem., TNO, Utrecht, Neth.
SO Organometallics in Chemical Synthesis (1970), Volume Date 1970-1971, 1,
57-68
CODEN: OMCSAW; ISSN: 0030-5162
DT Journal
LA English
CC 29 (Organometallic and Organometalloidal Compounds)
AB α -Functionally substituted organotin compds. R₃SnCH₂X add across the
carbonyl group of aldehydes and ketones R₁R₂C:O to give the corresponding
 β -triorganostannoxy-substituted-carbon-functional compds.
R₃SnOCR₁R₂CH₂X. Based on the observed substituent effects and on kinetic
measurements these reactions proceed by an ionic mechanism involving
nucleophilic attack on the carbonyl C atom as the rate-determining step. In
view of the ease of fission of the Sn-O bond of the stannoxy adducts by
mineral or organic acids (cleavage by malonic or oxalic acid is the preferred
method) this reaction offers an attractive route to
 β -hydroxysubstituted-carbon-functional compds. of the type
HOCR₁R₂CH₂X (R₁ = organic group or H). Starting from the appropriate
organotin nitriles (X = CN), esters (X = CO₂Et), ketones (X = Ac) and
amides (X = CONEt₂) a variety of β -hydroxynitriles, -esters, -ketones
and -amides were prepared NMR spectroscopy offers a useful tool to follow
the progress of the addition reactions. Representative NMR data for some
organotin adducts and for the corresponding
 β -hydroxy-substituted-carbon-functional compounds are given. The
synthesis of 18 new β -hydroxy compds. of the type HOCR₁R₂CH₂X is
presented as an example to illustrate the synthetic utility of this
reaction sequence.
ST tin org compd; Reformatskii reaction organotin

IT Aldehydes, reactions
Ketones, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(addition reaction of, with trialkylstannane derivs.)

IT Kinetics of addition reactions
(of carbonyl compds. with trialkylstannane derivs.)

IT Addition reactions
(of carbonyl compds. with trialkylstannane derivs., mechanism of)

IT 997-50-2D, Stannane, triethyl-, derivs. 14230-31-0 14230-36-5
17729-59-8 31602-69-4 31775-87-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(addition reaction of, with carbonyl compds.)

IT 1029-92-1 5381-93-1 17226-70-9 17981-09-8 17981-12-3 17981-13-4
17981-16-7 17981-17-8 17981-18-9 17981-25-8 19486-93-2
30543-30-7, 5-Hexen-2-one, 4-[(triethylstannyl)oxy]-
RL: PRP (Properties)
(nuclear magnetic resonance of)

IT 6050-51-7P 7466-48-0P 7497-61-2P 17981-24-7P 19487-29-7P
25290-13-5P 25290-14-6P, 2-Heptanone, 4-hydroxy- 25290-15-7P
25290-16-8P 25290-18-0P 25290-19-1P 25290-20-4P 25290-21-5P,
2-Furanhydracrylic acid, methyl ester 30543-15-8P, 2-Butanone,
4-(o-chlorophenyl)-4-hydroxy- 30543-21-6P, 2-Propanone,
1-(1-hydroxy-1-indanyl)- 30543-32-9P, Hydrocinnamic acid,
 β,β' -[(diethylstannylene)dioxy]bis-, dimethyl ester
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

REFERENCE 10

AN 71:101296 CA <<LOGINID::20081224>>
TI Alcohols
IN Cremers, Henricus M. J. C.; Noltes, Jan G.
PA Nederlandse Centrale Organisatie voor Toegepast-Natuurwetenschappelijk
Onderzoek
SO Ger. Offen., 22 pp.
CODEN: GWXXBX
DT Patent
LA German
IC C07BCD
CC 23 (Aliphatic Compounds)

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	----	-----	-----	-----
PI	DE 1816282		19690717	DE 1968-1816282	19681221
	NL 6800090			NL	
	NL 6816868			NL	
PRAI	NL	19680103			
	NL	19681126			

AB The title compds. were prepared by reacting an organotin compound with a ketone or thioketone followed by mild hydrolysis. Thus, 1.5 g. pentafluorobenzaldehyde was treated with Bu₃SnCH₂CN at room temperature 16 hrs. followed by addition of 2 ml. absolute Et₂O and 161 mg. HCl dissolved in absolute

Et₂O to give 63% C₆F₅CH(OH)CH₂CN, m. 88-9°. The following compds. were similarly prepared (comp. and properties given): Cl₃CCCH(OH)CH₂CO₂Et, m. 54.5-5.5°; PrCH(OH)CH₂COMe, b₀.04 40°, n₂₀D 1.4343; PhCH(OH)CH₂C(OH)Me, b₀.09 90-2°, n₂₀D 1.5264; p-O₂NC₆H₄CH(OH)CH₂C(O)Me, -; RCH(OH)CH₂COMe (R = 2-furyl), b₀.07 76-8°; n₂₀D 1.4923; (ClCH₂)₂C(OH)CH₂COMe, 61-2°, n₂₀D 1.4829; 1-acetylmethylcyclopentanol, b₀.03-0.05 48-b₀.05 50°; 1-acetylmethylcyclohexanol, n₂₀D 1.4701;

C13CCH(OH)CH2CONEt2, m. 63-5°; C6F5CH(OH)CH2C(O)NEt2, m.

66-7.5°; RCH(OH)CH2CO NEt2 (R = 2-furyl), b0.2

128-32°, n20D 1.5302; PhCMe(OH)C H2COMe, b0.07

68-78° n20D 1.5530; PhCH(OH)CH2CONEt2, n20D 1.5265;

N,N-diethyl-(1-hydroxycyclopentyl)acetamide, -; PhCH(OH)CH2CN, -;

RCH(OH)CH2CN (R = 2-furyl), -; RCH(OH)CH2CO2Et (R = 2-furyl), -; p-O2N

C6H4CH(OH)CH2CO2Et, -.

ST hydroxy ketone; ketone hydroxy; amides hydroxy; ester hydroxy; nitriles hydroxy; organo tins ketone; tins organo ketone

IT Alcohols, preparation

RL: PREP (Preparation)

(from carbonyl compds. by reaction with organic tin compds.)

IT Carbonyl compounds, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(with organic tin compds., alcs. by)

IT 38134-31-5P

RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation)

(Alcohols)

IT 5381-93-1P 6050-51-7P 7497-61-2P 15121-66-1P 17981-09-8P

17981-10-1P 17981-11-2P 17981-12-3P 17981-13-4P 17981-24-7P

19486-93-2P 19487-29-7P 25290-13-5P 25290-14-6P 25290-15-7P

25290-16-8P 25290-17-9P 25290-18-0P 25290-19-1P 25290-20-4P

25290-21-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

IT 7440-31-5, Tin

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of organic, with carbonyl compds.)

ACCESSION NUMBER: 142:429938 CA <<LOGINID::20081224>>

TITLE: Stereoselective catalytic hydrogenation process for the preparation of (S)- or (R)-4-halo-3-hydroxybutyrate esters from the corresponding 4-halo-3-oxobutyrate

PATENT ASSIGNEE(S): Lonza AG, Switz.

SOURCE: Eur. Pat. Appl., 9 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1528053	A1	20050504	EP 2003-24865	20031031
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
AU 2004291249	A1	20050602	AU 2004-291249	20041022
CA 2541716	A1	20050602	CA 2004-2541716	20041022
WO 2005049545	A1	20050602	WO 2004-EP11971	20041022
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1682481	A1	20060726	EP 2004-790763	20041022

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK
 CN 1874989 A 20061206 CN 2004-80032075 20041022
 BR 2004016133 A 20070102 BR 2004-16133 20041022
 JP 2007509874 T 20070419 JP 2006-537143 20041022
 KR 2006095769 A 20060901 KR 2006-708041 20060426
 NO 2006002131 A 20060530 NO 2006-2131 20060512
 IN 2006DN03081 A 20070810 IN 2006-DN3081 20060529
 US 20070078279 A1 20070405 US 2006-577385 20060703
 PRIORITY APPLN. INFO.: EP 2003-24865 20031031
 WO 2004-EP11971 20041022
 GI

/ Structure 10 in file .gra /

AB Optically active β -hydroxycarboxylate esters $R_1CH(OH)CH_2CO_2R_2$ [R_1 = C1-10 (un)branched perfluoroalkyl or perchloroalkyl; R_2 = C1-8 lower alkyl, (un)substituted benzyl; e.g., optically active Et 4,4,4-trifluoro-3-hydroxybutanoate] are prepared in high yield and selectivity by stereoselective hydrogen transfer to the corresponding β -ketocarboxylate esters $R_1COCH_2CO_2R_2$ (e.g., Et 4,4,4-trifluoro-3-oxobutanoate) in the presence of hydrogen donors (e.g., formic acid-triethylamine mixts.) and a chiral ruthenium-diamine complex catalyst [I; * = asym. carbon atom; R_3, R_4 = alkyl, Ph, (un)substituted cycloalkyl; R_5 = methanesulfonyl, trifluoromethanesulfonyl, benzenesulfonyl, (un)substituted naphthyl, camphorsulfonyl, alkoxy-carbonyl, (un)substituted benzoyl; R_6 = H, alkyl; A = (un)substituted aromatic compound; X = halogen; e.g., $RuCl[(1R,2R)\text{-p-TsNHCH(C}_6\text{H}_5\text{)CH(C}_6\text{H}_5\text{)NH}_2]$ (p-cymene)].
<http://www.cas.org/legal/infopolicy.html>

=> activate SA2577385/A
 L1 (1)SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON "ETHYL 4,4,4-TRICHLOR
 L2 1 SEA FILE=CAPLUS SPE=ON ABB=ON PLU=ON L1 AND HYDROGENATION

=> d ibib abs l2

L2 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2005:393998 CAPLUS <<LOGINID::20081229>>
 DOCUMENT NUMBER: 142:429938
 TITLE: Stereoselective catalytic hydrogenation
 process for the preparation of (S)- or
 (R)-4-halo-3-hydroxybutyrate esters from the
 corresponding 4-halo-3-oxobutyrate
 PATENT ASSIGNEE(S): Lonza AG, Switz.
 SOURCE: Eur. Pat. Appl., 9 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1528053	A1	20050504	EP 2003-24865	20031031
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
AU 2004291249	A1	20050602	AU 2004-291249	20041022
CA 2541716	A1	20050602	CA 2004-2541716	20041022

WO 2005049545 A1 20050602 WO 2004-EP11971 20041022
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
SN, TD, TG
EP 1682481 A1 20060726 EP 2004-790763 20041022
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK
CN 1874989 A 20061206 CN 2004-80032075 20041022
BR 2004016133 A 20070102 BR 2004-16133 20041022
JP 2007509874 T 20070419 JP 2006-537143 20041022
KR 2006095769 A 20060901 KR 2006-708041 20060426
NO 2006002131 A 20060530 NO 2006-2131 20060512
IN 2006DN03081 A 20070810 IN 2006-DN3081 20060529
US 20070078279 A1 20070405 US 2006-577385 20060703
PRIORITY APPLN. INFO.: EP 2003-24865 A 20031031
WO 2004-EP11971 W 20041022
OTHER SOURCE(S): CASREACT 142:429938; MARPAT 142:429938
GI
/ Structure 11 in file .gra /

AB Enantiomerically pure (S)- or (R)-4-halo-3-hydroxybutyrates [I; II; R1 = CH2X, CHX2, CX3; X = Cl and/or Br; R2 = C1-6 alkyl, C3-8 cycloalkyl, (un)substituted aryl, (un)substituted aralkyl; e.g., Et (3S)-4-chloro-3-hydroxybutyrate] are prepared in high yield and selectivity by the asym. hydrogenation of 4-halo-3-oxobutyrate esters R1C(:O)CH2CO2R2 (e.g., Et 4-chloro-3-oxobutyrate) in the presence of a catalyst of a ruthenium complex comprising a chiral diphosphine ligand (III).

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> activate SA577385/A
L3 (1)SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON "4,4,4-TRIFLUORO-3-OX
L4 (1)SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON "4-CHLORO-3-OXOBUTANO
L5 (40)SEA FILE=CAPLUS SPE=ON ABB=ON PLU=ON L4 AND L3
L6 8 SEA FILE=CAPLUS SPE=ON ABB=ON PLU=ON L5 AND HYDROGENATION

=> d ibib abs 16 1-8

L6 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:362416 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 148:121227
TITLE: Ruthenium catalyzed asymmetric hydrogenation
of α - and β -ketoesters in room temperature
ionic liquids using chiral P-Phos ligand
AUTHOR(S): Xu, Lijin; Lam, Kim Hung; Ruan, Jiwu; Fan, Qinghua;
Chan, Albert S. C.
CORPORATE SOURCE: Open Laboratory of Chirrotechnology of the Institute of
Molecular Technology for Drug Discovery and Synthesis
and Department of Applied Biology and Chemical
Technology, The Hong Kong Polytechnic University, Hong

Kong, Peop. Rep. China
SOURCE: ACS Symposium Series (2007), 950(Ionic Liquids in
Organic Synthesis), 224-234
CODEN: ACSMC8; ISSN: 0097-6156
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 148:121227
AB Chiral dipyridyl phosphine ligand was found to be effective in the
Ru-catalyzed asym. hydrogenation of α - and β -keto
esters in room temperature ionic liqs. with high conversions and good to
excellent enantioselectivities.
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:37762 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 144:273900
TITLE: Multigram-scale asymmetric hydrogenation
reactions using Ru-SYNPHOS and Ru-DIFLUORPHOS
catalysts
AUTHOR(S): Jeulin, Severine; Champion, Nicolas; Dellis, Philippe;
Ratovelomanana-Vidal, Virginie; Genet, Jean-Pierre
CORPORATE SOURCE: Laboratoire de Synthese Selective Organique et
Produits Naturels (UMR 7573 CNRS), Ecole Nationale
Superieure de Chimie de Paris, Paris, 75231/05, Fr.
SOURCE: Synthesis (2005), (20), 3666-3671
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:273900
AB The detailed procedure for the synthesis of Ru-SYNPHOS and Ru-DIFLUORPHOS
catalysts are described. These catalysts displayed high rates and are
quite effective for the large-scale hydrogenation reactions of
carbonyl compds., such as β -keto esters RCOCH₂CO₂Et (R = Me, ClCH₂,
F₃C, Ph, PhCH₂OCH₂), acetylacetone and hydroxyacetone.
REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1206596 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 144:107747
TITLE: Ruthenium catalyzed asymmetric hydrogenation
of α - and β -keto esters in ionic liquids
using chiral P-Phos ligand
AUTHOR(S): Lam, Kim Hung; Xu, Lijin; Feng, Lichun; Ruan, Jiwu;
Fan, Qinghua; Chan, Albert S. C.
CORPORATE SOURCE: Open Laboratory of Chirotechnology of the Institute of
Molecular Technology for Drug Discovery and Synthesis
and Department of Applied Biology and Chemical
Technology, The Hong Kong Polytechnic University, Hong
Kong, Peop. Rep. China
SOURCE: Canadian Journal of Chemistry (2005), 83(6-7), 903-908
CODEN: CJCHAG; ISSN: 0008-4042
PUBLISHER: National Research Council of Canada
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:107747
AB Chiral dipyridylphosphine ligand was used in the Ru-catalyzed asym.
hydrogenation of α - and β -keto esters in room temperature

ionic liqs. giving the corresponding α - and β -hydroxy esters with high conversions and good to excellent enantioselectivities. The catalyst was recycled by simple extraction and reused five times without loss of activity and enantioselectivity.

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:626146 CAPLUS <<LOGINID::20081229>>

DOCUMENT NUMBER: 141:313992

TITLE: New developments in the synthesis of heterotopic atropisomeric diphosphines via diastereoselective aryl coupling reactions

AUTHOR(S): Madec, Jonathan; Michaud, Guillaume; Genet, Jean-Pierre; Marinetti, Angela

CORPORATE SOURCE: Laboratoire de Synthèse Selective Organique et Produits Naturels, UMR 7573, ENSCP 11, Paris, 75231, Fr.

SOURCE: Tetrahedron: Asymmetry (2004), 15(14), 2253-2261
CODEN: TASYE3; ISSN: 0957-4166

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:313992

AB The new heterotopic atropisomeric diphosphine (R)-5,6-benzo-2,2'-bis(diphenylphosphino)-4',5',6'-trimethylbiphenyl has been prepared. The key step of this synthesis is a diastereoselective, intramol. aryl-aryl coupling reaction via oxidation of a suitable, chiral diarylcuprate. The catalytic properties of the diphosphine in ruthenium promoted hydrogenations of model substrates and in rhodium promoted 1,4-addns. of boronic acids to α,β -unsatd. ketones are fully comparable to those of reference ligands such as BINAP. This seems to indicate that C2-symmetry is not a structural prerequisite for atropisomeric chiral diphosphines to obtain high enantioselectivities in 1,4-addition reactions as well as in hydrogenation reactions.

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:356392 CAPLUS <<LOGINID::20081229>>

DOCUMENT NUMBER: 141:71622

TITLE: Chiral biphenyl diphosphines for asymmetric catalysis: stereoelectronic design and industrial perspectives

AUTHOR(S): Jeulin, Severine; De Paule, Sebastien Duprat; Ratovelomanana-Vidal, Virginie; Genet, Jean-Pierre; Champion, Nicolas; Dellis, Philippe

CORPORATE SOURCE: Laboratoire de Synthèse Selective Organique et Produits Naturels, Ecole Nationale Supérieure de Chimie de Paris, Paris, 75231, Fr.

SOURCE: Proceedings of the National Academy of Sciences of the United States of America (2004), 101(16), 5799-5804
CODEN: PNASA6; ISSN: 0027-8424

PUBLISHER: National Academy of Sciences

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:71622

GI

/ Structure 12 in file .gra /

AB Both enantiomers of the chiral diphosphines I (SYNPHOS) and II (DIFLUORPHOS) are prepared on multigram scales; the electronic and steric characteristics of I and II and of rhodium complexes derived from them are determined, compared with previous diphosphine catalysts, and correlated with their activities and enantioselectivities in the hydrogenation of ketones and olefins. I and II are prepared in five steps from 6-bromo-2,3-dihydro-1,4-benzodioxane and 5-bromo-2,2-difluorobenzodioxole, resp.; lithium-metal exchange and addition to a phosphoryl or phosphinyl chloride followed by oxidation to yield phosphine oxides, regioselective lithiation and iodination, Ullman coupling of the aryl iodides, resolution (either by acid-base resolution with di-O-benzoyl-tartaric acid or by chiral HPLC), and reduction of the phosphine oxides yields I and II in 38% and 33% overall yield, resp. The bite angles of I and II are compared to those of other common diphosphine ligands such as BINAP and MeO-BIPHEP. The structure of diastereomeric chlorohydridoruthenium complexes of (S)-II with Me acetoacetate is determined. The C-O stretching frequencies of chloro(carbonyl)rhodium diphosphine complexes containing I, II, BINAP, and MeO-BIPHEP are determined as a measure of the electronic demands of the diphosphine ligands. β -Keto ester, α -keto ester, 1,3-diketone, ketone, and olefin substrates are hydrogenated in the presence of nonracemic I, II, BINAP, and MeO-BIPHEP and bis(η^3 -methallyl)(η^4 -1,5-cyclooctadienyl)ruthenium; the enantioselectivities are correlated with the steric and electronic properties of the ligands. The stereoelectronic features of the ligand and the substrate deeply influence the enantioselectivities obtained in asym. hydrogenation; whereas the steric and electronic factors for I (as in other diphosphines) correlate well, the bite angle of II does not correlate to its electronic effects in asym. hydrogenation reactions, leading to complementary hydrogenation selectivities for ligands I and II.

REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:70307 CAPLUS <<LOGINID::20081229>>

DOCUMENT NUMBER: 140:253116

TITLE: Difluorophos, an electron-poor diphosphane: A good match between electronic and steric features

AUTHOR(S): Jeulin, Severine; Duprat de Paule, Sebastien; Ratovelomanana-Vidal, Virginie; Genet, Jean-Pierre; Champion, Nicolas; Dellis, Philippe

CORPORATE SOURCE: Laboratoire de Synthese Selective Organique et Produits Naturels, Ecole Nationale Supérieure de Chimie de Paris, Paris, 75231, Fr.

SOURCE: Angewandte Chemie, International Edition (2004), 43(3), 320-325

CODEN: ACIEF5; ISSN: 1433-7851

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:253116

GI

/ Structure 13 in file .gra /

AB Both enantiomers of difluorophos I were synthesized and their stereoelectronic features were evaluated in theor. and exptl. studies. The unusual π acidity of I explains the excellent results obtained with it in ruthenium-mediated asym. hydrogenation of fluorinated β -functionalized ketones. These results are better than those obtained with other biphenyl-based diphosphines.

REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1994:502611 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 121:102611
ORIGINAL REFERENCE NO.: 121:18339a,18342a
TITLE: purification and characterization of a novel carbonyl reductase isolated from Rhodococcus erythropolis
AUTHOR(S): Zelinski, Thomas; Peters, Joerg; Kula, Maria-Regina
CORPORATE SOURCE: Institut fuer Enzymtechnologie der Heinrich-Heine-Universitaet Duesseldorf, Forschungszentrum Juelich (KFA), Julich, 52404, Germany
SOURCE: Journal of Biotechnology (1994), 33(3), 283-92
CODEN: JBITD4; ISSN: 0168-1656
DOCUMENT TYPE: Journal
LANGUAGE: English

AB During growth on n-tetradecane a novel NADH-dependent carbonyl reductase is induced in the Gram-pos. bacterium Rhodococcus erythropolis (Peters, P., Zelinski, T. and Kula, M.R. (1992) Appl. microbiol. biotechnol. 38, 334-340). The enzyme has been purified to homogeneity using fractional pH precipitation, anion exchange chromatog. and affinity chromatog. The isoelec. point of the oxidoreductase is 4.4. The apparent mol. mass of the native enzyme is 161 kDa, that of the subunits 40 kDa as determined by SDS gel electrophoresis. A tetrameric structure of the carbonyl reductase is consistent with these results. Important biochem. data concerning the application of the reductase are: a broad pH-optimum, temperature optimum at 40° and stability at room temperature for more than 5 days. The oxidoreductase accepted as substrate aliphatic and aromatic ketones, keto esters (esters of keto carboxylic acids) and halogenated carbonyl compds. and reduced them to the corresponding hydroxyl compds. with (S)-configuration with more than 98% enantiomeric excess. The NAD+-dependent oxidation of primary alcs. was not catalyzed by the carbonyl reductase, whereas secondary alcs. and hydroxy acid esters were oxidized to the corresponding carbonyl compds. at about 10-fold slower reaction rates compared to the reduction

L6 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1993:603787 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 119:203787
ORIGINAL REFERENCE NO.: 119:36369a,36372a
TITLE: Stereodivergent synthesis of fluorinated threonine derivatives in high optical purity
AUTHOR(S): Shimizu, Makoto; Yokota, Tetsuya; Fujimori, Kouichi; Fujisawa, Tamotsu
CORPORATE SOURCE: Dep. Chem. Mater., Mie Univ., Tsu, 514, Japan
SOURCE: Tetrahedron: Asymmetry (1993), 4(5), 835-8
CODEN: TASYE3; ISSN: 0957-4166
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 119:203787

AB Fluorinated 3-acetoxy-2-(methoxyimino)butyrates were resolved by lipase to

give the corresponding alcs. and the acetates in high optical purity. The resolved alcs. were readily converted into mono-, di-, and trifluorothreonine and allothreonine derivs. by hydrogenation of the methoxyimino group.

<http://www.cas.org/support/stngen/stdoc/properties.html>

=> e "ethyl 4-bromo-3-oxobutanoate"/cn

E1	1	ETHYL 4-BROMO-3-METHYLTHIOPHENE-2-CARBOXYLATE/CN
E2	1	ETHYL 4-BROMO-3-NITROBENZOATE/CN
E3	1 -->	ETHYL 4-BROMO-3-OXOBUTANOATE/CN
E4	1	ETHYL 4-BROMO-3-OXOBUTANOATE, COPPER COMPLEX/CN
E5	1	ETHYL 4-BROMO-3-OXOBUTYRATE/CN
E6	1	ETHYL 4-BROMO-3-OXOCYCLOHEXANECARBOXYLATE/CN
E7	1	ETHYL 4-BROMO-3-OXOHEPTANOATE/CN
E8	1	ETHYL 4-BROMO-3-OXOHEXANOATE/CN
E9	1	ETHYL 4-BROMO-3-OXONONANOATE/CN
E10	1	ETHYL 4-BROMO-3-OXOPENTANOATE/CN
E11	1	ETHYL 4-BROMO-3-OXOVALERATE/CN
E12	1	ETHYL 4-BROMO-3-PROPYLHEPTANOATE/CN

=> e "ethyl 4-bromo-3-hydroxybutanoate"/cn

E1	1	ETHYL 4-BROMO-3-ETHOXYCROTONATE/CN
E2	1	ETHYL 4-BROMO-3-HYDROXYBENZOATE/CN
E3	1 -->	ETHYL 4-BROMO-3-HYDROXYBUTANOATE/CN
E4	1	ETHYL 4-BROMO-3-HYDROXYBUTYRATE/CN
E5	1	ETHYL 4-BROMO-3-HYDROXYCYCLOHEXANECARBOXYLATE/CN
E6	1	ETHYL 4-BROMO-3-HYDROXYPIPERIDINE-1-CARBOXYLATE/CN
E7	1	ETHYL 4-BROMO-3-METHOXY-2-PENTENOATE/CN
E8	1	ETHYL 4-BROMO-3-METHOXYCROTONATE/CN
E9	1	ETHYL 4-BROMO-3-METHOXYPHENOXYACETATE/CN
E10	1	ETHYL 4-BROMO-3-METHOXYTHIOFURAN-2-CARBOXYLATE/CN
E11	1	ETHYL 4-BROMO-3-METHOXYTHIOPHENE-2-CARBOXYLATE/CN
E12	1	ETHYL 4-BROMO-3-METHYL-2-BUTENOATE/CN

=> s e3

L7 1 "ETHYL 4-BROMO-3-HYDROXYBUTANOATE"/CN

=> d l7 ide

L7 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN

RN 32224-01-4 REGISTRY

ED Entered STN: 16 Nov 1984

CN Butanoic acid, 4-bromo-3-hydroxy-, ethyl ester (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Butyric acid, 4-bromo-3-hydroxy-, ethyl ester (7CI, 8CI)

OTHER NAMES:

CN (±)-Ethyl 4-bromo-3-hydroxybutyrate

CN 4-Bromo-3-hydroxybutanoic acid ethyl ester

CN Ethyl γ-bromo-β-hydroxybutyrate

CN Ethyl 4-bromo-3-hydroxybutanoate

CN Ethyl 4-bromo-3-hydroxybutyrate

DR 128052-98-2

MF C6 H11 Br O3

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

/ Structure 14 in file .gra /

<http://www.cas.org/legal/infopolicy.html>

=> s l7

L9 17 L7

=> d 19 ibib abs 1-17

L9 ANSWER 1 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2008:974948 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 149:268051
TITLE: Preparation of benzimidazole, benzothiazole and
benzoxazole derivatives and their use as LTA4
hydrolase modulators
INVENTOR(S): Barchuk, William T.; Dunford, Paul J.; Edwards, James
P.; Fourie, Anne M.; Karlsson, Lars; Quan, Joanne M.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 140pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20080194630	A1	20080814	US 2008-69943	20080214
WO 2008100564	A1	20080821	WO 2008-US1949	20080214
W:	AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			

PRIORITY APPLN. INFO.: US 2007-889851P P 20070214

OTHER SOURCE(S): MARPAT 149:268051

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. I and related phenethylamine and phenoxyethylamine analogs are disclosed [X = NH, NMe, O, S; Y = CH₂, O; R₄ = H, OMe, Cl, F, Br, I, OH, NH₂, CN, CF₃, Me; R₆ = H, F; R₂, R₃ = independently alk(en/yn)yl, SO₂-alkyl, alkylheteroaryl; or NR₂R₃ = (un)substituted heterocyclyl]. Leukotriene A₄ hydrolase (LTA₄H) inhibitors of formula I, including their enantiomers, diastereomers, racemics, tautomers, hydrates, solvates or pharmaceutically acceptable salts, esters, or amides, compns. containing them, and their use for the treatment, prevention or inhibition of inflammation and/or conditions associated with inflammation are disclosed. For example, II was prepd, in 63% yield, by amination of 2-[4-(2-bromoethoxy)phenoxy]benzothiazole (preparation given) with 1-(piperidin-4-yl)pyrrolidin-2-one hydrochloride. II displayed a IC₅₀ of 1 nM in a recombinant human LTA₄ hydrolase assay.

L9 ANSWER 2 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:873237 CAPLUS <<LOGINID::20081229>>

DOCUMENT NUMBER: 147:277913
 TITLE: Improved method and kit for automated resolving agents, especially amino acid derivatives, and solvents selection
 INVENTOR(S): Vaidya, Niteen A.
 PATENT ASSIGNEE(S): USA
 SOURCE: U.S. Pat. Appl. Publ., 29pp.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20070185346	A1	20070809	US 2006-347532	20060203
WO 2007092264	A2	20070816	WO 2007-US2800	20070131
WO 2007092264	A3	20071129		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA				
EP 1981831	A2	20081022	EP 2007-763121	20070131
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
PRIORITY APPLN. INFO.:			US 2006-347532	A2 20060203
			WO 2007-US2800	W 20070131

AB The invention is related to a kit for improved identification of the optimal conditions for diastereomeric salt crystallization and the selection of the optimal resolving agents, especially amino acid derivs., and solvents, which

include A. an array of containers wherein the array is a standard high throughput tray and the containers are a multiplicity of substantially identical containers or well plates each optionally sealed with a sealant or stoppers to avoid loss of chemical solvent; B. wherein each substantially identical container has a unique combination of resolving agent in each column and at least one suitable solvent in each row; and C. an instructional text to use said kit. The tray of 24, 48, 96 or more samples is examined simultaneously visually or by standard anal. techniques. Resolution of (+)-2-phenylpropionic acid was studied with both amines and acids as resolving agents. Strychnine in 96% ethanol was ideal system for (+)-isomer, while quinidine in 96% ethanol was the system of choice for (-)-isomer. Pyroglutamic acid in 70% isopropanol was ideal system for (+)-isomer, while malic acid in 1-butanol was the system of choice for (-)-isomer.

L9 ANSWER 3 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2006:1267800 CAPLUS <<LOGINID::20081229>>
 DOCUMENT NUMBER: 146:242727
 TITLE: Enantiomeric impurities in chiral synthons, catalysts, and auxiliaries: Part 3
 AUTHOR(S): Huang, Ke; Breitbach, Zachary S.; Armstrong, Daniel W.
 CORPORATE SOURCE: Department of Chemistry and Biochemistry, University

SOURCE: of Texas at Arlington, Arlington, TX, 76019, USA
Tetrahedron: Asymmetry (2006), 17(19), 2821-2832
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The enantiomeric excess of chiral reagents used in asym. syntheses directly affects the reaction selectivity and product purity. Eighty-four of the more recently available chiral compds. were evaluated to determine their actual enantiomeric composition. These compds. are widely used in asym. syntheses as chiral synthons, catalysts, and auxiliaries. These include chiral alcs., amines, amino alcs., amides, carboxylic acids, epoxides, esters, ketones, and oxolanes among other classes of compds. All enantiomeric test results were categorized within five impurity levels (i.e., <0.01%, 0.01-0.1%, 0.1-1%, 1-10%, and >10%). The majority of the reagents tested have enantiomeric impurities over 0.01%, and two of them contain enantiomeric impurities exceeding the 10% level. The most effective enantioselective anal. method was a GC approach using a Chiraldex GTA chiral stationary phase (CSP). This method worked exceedingly well with chiral amines and alcs.

REFERENCE COUNT: 121 THERE ARE 121 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 4 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:1240791 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 143:476533
TITLE: The method of making optically active ester derivatives and their acids from racemic esters
INVENTOR(S): Chung, Sun Ho; Hwang, Soon Ook
PATENT ASSIGNEE(S): Enzytech, Ltd., S. Korea
SOURCE: PCT Int. Appl., 12 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005111227	A1	20051124	WO 2005-KR1213	20050427
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
KR 2005104481	A	20051103	KR 2004-29791	20040429
EP 1740714	A1	20070110	EP 2005-764804	20050427
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
CN 1946855	A	20070411	CN 2005-80013419	20050427
US 20080038802	A1	20080214	US 2006-587228	20061023
PRIORITY APPLN. INFO.:				
			KR 2004-29791	A 20040429
			WO 2005-KR1213	W 20050427
OTHER SOURCE(S): MARPAT 143:476533				

AB The present invention relates to process for the preparing of optically active ester derivs. and their acid derivs. which are used intensively as important chiral intermediates from racemic β -hydroxybutyl ester derivs. In more detail, this invention relates to the process for preparing optically active β -hydroxybutyl ester derivs. and their acid derivs. by stereospecific hydrolysis of racemic β -hydroxybutyl ester derivs. using lipases or lipase-producing microorganisms in the aqueous phase or organic phase including aqueous solvent. The method of making optically active ester derivs. and their acid derivs. by hydrolysis of β -hydroxybutyl ester derivs. is easier and more economical than conventional methods and the products have high optical purity. Also, separation of ester derivs. from acid derivs. is easy after reaction. Thus, this method is a useful process on the industrial scale.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 5 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:120925 CAPLUS <<LOGINID::20081229>>

DOCUMENT NUMBER: 142:219285

TITLE: Preparation of benzimidazole, benzothiazole and benzoxazole derivatives and their use as LTA4 hydrolase modulators

INVENTOR(S): Axe, Frank U.; Bembenek, Scott D.; Butler, Christopher R.; Edwards, James P.; Fourie, Anne M.; Grice, Cheryl A.; Savall, Brad M.; Tays, Kevin L.; Wei, Jianmei

PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.

SOURCE: PCT Int. Appl., 390 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005012296	A1	20050210	WO 2004-US24050	20040727
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004261610	A1	20050210	AU 2004-261610	20040727
CA 2534212	A1	20050210	CA 2004-2534212	20040727
US 20050043378	A1	20050224	US 2004-900103	20040727
US 20050043379	A1	20050224	US 2004-900152	20040727
EP 1660491	A1	20060531	EP 2004-779219	20040727
EP 1660491	B1	20080806		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
BR 2004013072	A	20061003	BR 2004-13072	20040727
CN 1856490	A	20061101	CN 2004-80027906	20040727
JP 2007500703	T	20070118	JP 2006-521973	20040727
SG 129449	A1	20070226	SG 2007-691	20040727
SG 130192	A1	20070320	SG 2007-817	20040727
AT 403654	T	20080815	AT 2004-779219	20040727

AT 405562	T	20080915	AT 2004-779375	20040727
MX 2006PA01122	A	20060907	MX 2006-PA1122	20060127
KR 2006054408	A	20060522	KR 2006-702211	20060131
NO 2006000823	A	20060315	NO 2006-823	20060220
PRIORITY APPLN. INFO.:			US 2003-490710P	P 20030728
			WO 2004-US24050	W 20040727
OTHER SOURCE(S):	CASREACT 142:219285; MARPAT 142:219285			
GI				

L9 ANSWER 6 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2005:55193 CAPLUS <<LOGINID::20081229>>
 DOCUMENT NUMBER: 142:155558
 TITLE: Cyanation method for producing
 4-cyano-3-hydroxybutyric acid esters from their
 corresponding 4-leaving-group-substituted derivatives
 and cyanide salts
 INVENTOR(S): Eckert, Markus; Rodefelf, Lars; Brackemeyer, Thomas;
 Dreisbach, Claus; Rampf, Florian; Schlummer, Bjoern
 PATENT ASSIGNEE(S): Bayer Chemicals AG, Germany
 SOURCE: PCT Int. Appl., 20 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2005005375	A1	20050120	WO 2004-EP7030	20040629
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10331211	A1	20050127	DE 2003-10331211	20030710
PRIORITY APPLN. INFO.:			DE 2003-10331211	A 20030710
OTHER SOURCE(S):	CASREACT 142:155558; MARPAT 142:155558			
AB 4-Cyano-3-hydroxybutyric acid esters (e.g., Et 4-cyano-3-hydroxybutyrate) are prepared by the cyanation-substitution reaction of 4-leaving-group-substituted-3-hydroxybutyric acid esters (e.g., Et 4-chloro-3-hydroxybutyrate) with a cyanide salt (e.g., sodium cyanide) in an organic solvent (formamide) in the presence of one or several other salts (sodium dihydrogenphosphate).				
REFERENCE COUNT:	3	THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT		

L9 ANSWER 7 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2004:308406 CAPLUS <<LOGINID::20081229>>
 DOCUMENT NUMBER: 140:321018
 TITLE: Process for the preparation of a lower alkyl
 4-cyano-3-hydroxybutyrate from
 3-hydroxy- γ -butyrolactone
 INVENTOR(S): Kwon, Taesoo; Gu, Chen; Yang, Soon-Ha
 PATENT ASSIGNEE(S): SK Energy and Chemical Inc., USA

SOURCE: PCT Int. Appl., 11 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004031131	A1	20040415	WO 2003-US30869	20030930
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2500668	A1	20040415	CA 2003-2500668	20030930
AU 2003272793	A1	20040423	AU 2003-272793	20030930
EP 1551796	A1	20050713	EP 2003-754994	20030930
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1688539	A	20051026	CN 2003-823536	20030930
JP 2006502201	T	20060119	JP 2004-541917	20030930
IN 2005DN01239	A	20070119	IN 2005-DN1239	20050330
PRIORITY APPLN. INFO.:			US 2002-415672P	P 20021003
			WO 2003-US30869	W 20030930

OTHER SOURCE(S): CASREACT 140:321018

AB Alkyl 4-cyano-3-hydroxybutyrates are prepared by: (a) reacting 3-hydroxy- γ -butyrolactone using a haliding reagent in the presence of an acylating agent in a lower alkanol solvent so as to provide a reaction product comprising a lower alkyl 4-halo-3-hydroxybutyrate (halo = bromo, iodo); and (b) reacting the reaction product from step (a), without isolation or purification, with a source of cyanide ion (e.g., NaOH) in a reaction mixture having a pH of 7-11 to produce a lower alkyl 4-cyano-3-hydroxybutyrate (ACHB) with minimal byproduct formation.

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 8 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:935084 CAPLUS <<LOGINID::20081229>>

DOCUMENT NUMBER: 138:253757

TITLE: The enantioselectivity of reduction of ethyl 4-halo-3-oxobutanoate catalyzed by *Geotrichum candidum* depends on the cofactor

AUTHOR(S): Sundby, Eirik; De Zotti, Marta; Anthonsen, Thorleif

CORPORATE SOURCE: Department of Chemistry, Norwegian University of Science and Technology, Trondheim, N-7491, Norway

SOURCE: Journal of Molecular Catalysis B: Enzymatic (2003), 21(1-2), 63-66

CODEN: JMCEF8; ISSN: 1381-1177

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:253757

AB Enantioselective redns. of Et 3-oxobutanoates with fermenting cells or acetone treated cells of *Geotrichum candidum* gave 3-hydroxyesters with different ee and different predominant configurations depending on

reaction conditions. Et 4-bromo-3-oxobutanoate was reduced with APG4 and NADH to give predominantly Et (R)-4-bromo-3 hydroxybutanoate while the (S)-configuration was predominant when NADPH was the cofactor. Moreover, when the catalyst was heated before the reaction, the ee was increased indicating that the enzyme giving the (S)-alc. is more thermolabile than the other.

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 9 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:268357 CAPLUS <<LOGINID::20081229>>

DOCUMENT NUMBER: 120:268357

ORIGINAL REFERENCE NO.: 120:47523a,47526a

TITLE: Manufacture of (S)-gamma-halogenated-beta-hydroxybutyric acid esters for pharmaceutical synthesis

INVENTOR(S): Oonishi, Ikumasa; Shimaoka, Megumi; Kira, Ikuo; Nakazawa, Masakazu

PATENT ASSIGNEE(S): Ajinomoto KK, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06038776	A	19940215	JP 1993-85938	19930413
JP 3163338	B2	20010508		
US 5413921	A	19950509	US 1993-66239	19930525
PRIORITY APPLN. INFO.:			JP 1992-137111	A1 19920528

AB The title compds. are prepared by reducing γ -halogenated acetoacetates asym. by microorganisms such as Stemphylium, Alternaria, Corynespora, Preussia, Neurospora, Kabatiella, Gelasinospora, Neocosmospora, Sporormiella, Torulaspora, Pachysolen, and Sterigumatomyces. These compds. are starting materials for pharmaceutical synthesis.

L9 ANSWER 10 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:438920 CAPLUS <<LOGINID::20081229>>

DOCUMENT NUMBER: 113:38920

ORIGINAL REFERENCE NO.: 113:6617a,6620a

TITLE: Manufacture of L-carnitine chloride with lipase

INVENTOR(S): Horinaka, Akio

PATENT ASSIGNEE(S): Earth Chemical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02027995	A	19900130	JP 1988-177373	19880715
PRIORITY APPLN. INFO.:			JP 1988-177373	19880715

AB The title compound (I), useful in treatment of heart diseases, is manufactured by

transesterification of XCH₂CH(OH)CH₂Y (II, X = Cl, Br, I; Y = CN, alkoxy carbonyl) with lipase in the presence of fatty acid esters, separation of L-II, and conversion of them into I. II (X = Cl, Y = CN (III)) 4.78 and

9.88 g 2,2,2-trichloroethyl caproate were treated with lipase adsorbed on celite in ether at room temperature for 4 days and purified by silica gel column chromatog. to give 2.29 g unreacted III, which was treated with 30% trimethylamine aqueous solution at 4° overnight to afford 0.83 g L-carnitinenitrile. Treatment of the nitrile (0.8 g) with concentrated HCl at 90° for 4 h gave 0.67 g I.

L9 ANSWER 11 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:178661 CAPLUS <<LOGINID::20081229>>
 DOCUMENT NUMBER: 112:178661
 ORIGINAL REFERENCE NO.: 112:30213a,30216a
 TITLE: Preparation of 1-benzyl-4-hydroxy-2-pyrrolidinone as an intermediate for drugs and agrochemicals
 INVENTOR(S): Kutsuki, Hidetoshi; Maemoto, Shunichi; Hasegawa, Junzo
 PATENT ASSIGNEE(S): Kanegafuchi Chemical Industry Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01254658	A	19891011	JP 1988-83630	19880404
PRIORITY APPLN. INFO.:			JP 1988-83630	19880404

AB The title compound was prepared by treatment of 4-halo-3-hydroxybutyric esters with PhCH₂NH₂ (I), its salts, or their mixture ClCH₂CH(OH)CH₂CO₂Et and II in EtOH were refluxed 50 h with Na₂CO₃ to give 63% I.

L9 ANSWER 12 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:157695 CAPLUS <<LOGINID::20081229>>
 DOCUMENT NUMBER: 112:157695
 ORIGINAL REFERENCE NO.: 112:26651a,26654a
 TITLE: Preparation of optically active 4-halo-3-hydroxybutyric acid esters and carnitine
 INVENTOR(S): Noyori, Ryoji; Kitamura, Masahito; Okuma, Takeshi; Kumobayashi, Hidenori
 PATENT ASSIGNEE(S): Takasago Perfumery Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01211551	A	19890824	JP 1988-37032	19880219
JP 06078277	B	19941005		
EP 339764	A1	19891102	EP 1989-301585	19890217
EP 339764	B1	19920624		
R: CH, DE, FR, GB, IT, LI, NL				
US 4895979	A	19900123	US 1989-313007	19890221
PRIORITY APPLN. INFO.:			JP 1988-37032	A 19880219
OTHER SOURCE(S):			CASREACT 112:157695; MARPAT 112:157695	

GI

/ Structure 17 in file .gra /

AB XCH₂CH(OH)CH₂CO₂R (I; R = lower alkyl; X = Cl, Br) are prepared by asym. hydrogenation of XCH₂COCH₂CO₂R (II) in the presence of Ru₂Cl₄L₂Net₃ (L = Q; R₁ = H, Me, CMe₃), Ru(OCOR₂)₂L (R₂ = lower alkyl, CF₃), or RuX₂L at 70-150° and carnitine (III) is prepared by treatment of I with Me₃N without isolation. A mixture of II (R = Et, X = Cl), EtOH, and RuBr₂L [L = (-)-Q, R₁ = H] was autoclaved under 100 kg/cm² H at 100° for 10 min to give 97% (3R)-(+)-I (R = Et, X = Cl) with 97.2% e.e, vs. 47.0% and 67.0% e.e., resp., for a control using RuBr₂L [L = (+)-Q, Q₁ = H] at 19° for 16 h. A mixture of II (R = Me, X = Cl), MeOH, and Ru(OAc)₂L [L = (-)-Q, R₁ = H] was autoclaved under 100 kg/cm² H at 100° for 15 min, after distillation out MeOH and addition of an aqueous Me₃N solution, the reaction mixture was further stirred at 70° for 1.5 h and at 90° for 30 min to give 46% III.Cl.

L9 ANSWER 13 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1989:191289 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 110:191289
ORIGINAL REFERENCE NO.: 110:31739a,31742a
TITLE: Enzymic manufacture of γ -substituted β -hydroxybutyrate esters as intermediates for carnitine synthesis
INVENTOR(S): Yamada, Hideaki; Shimizu, Akira; Miyoshi, Teruzo; Kato, Masaaki; Morikawa, Tadashi
PATENT ASSIGNEE(S): Denki Kagaku Kogyo K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63309195	A	19881216	JP 1987-145587	19870611
JP 2566962	B2	19961225		

PRIORITY APPLN. INFO.: JP 1987-145587 19870611

AB The title compds., useful as intermediates for carnitine synthesis, are manufactured by treatment of γ -substituted acetoacetate esters with reducing enzymes in aqueous solvents in the presence of organic solvents which form two phases with H₂O. *Sporobolomyces salmonicolor* IFO 1038 was cultured in a medium containing glucose and corn steep liquor at 28° for 2 days, shake-cultured in the same medium at 28° for 4 days, and centrifuged to collect the bacteria. The bacteria were lysed by sonication in 0.01M phosphate buffer and treated with Et γ -chloroacetoacetate, NADPH, and AcOEt at 30° and pH 8 for 20 h under stirring to produce 92% Et γ -chloro- β -hydroxybutyrate, vs. 52% in the absence of AcOEt.

L9 ANSWER 14 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1987:32369 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 106:32369
ORIGINAL REFERENCE NO.: 106:5415a,5418a
TITLE: Asymmetric reduction of β -keto esters
INVENTOR(S): Ai, Kenzo
PATENT ASSIGNEE(S): Ajinomoto Co., Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.

CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61155354	A	19860715	JP 1984-281337	19841227
PRIORITY APPLN. INFO.:			JP 1984-281337	19841227

AB R1COCH2CO2R2 (R1, R2 = alkyl, alkenyl, alkynyl, aryl, aralkyl, etc.) are asym. reduced in the presence of [R3NR5CHR4(CH2)mY]n (R3, R5 = H, amino-protecting group, R3R5N = heterocycle; R4 = CO2H, CH2OH; m = 0-3; Y = SH, OH, NH2, CO2H when n = 1; Y = S when n = 2) and C1-20 alcs., PhOH, benzyl alc. etc. Thus, LiBH4 was added to a solution of 1.21 mmol (R,R)-N,N'-dibenzoylcystine and 1.61 mmol Me3COH in THF, refluxed, cooled, 1.01 mmol PhCOCH2CO2Et added, and the mixture stirred at -30° to give 94% (R)-(+)-PhCH(OH)CH2CO2Et of 87% optical yield.

L9 ANSWER 15 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1978:50233 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 88:50233
ORIGINAL REFERENCE NO.: 88:7917a,7920a
TITLE: Studies on ketene and its derivatives. LXXXV.
Reactions of 4-bromo-3-hydroxybutanoate and its acyl derivatives

AUTHOR(S): Kato, Tetsuzo; Kimura, Hitoshi
CORPORATE SOURCE: Pharm. Inst., Tohoku Univ., Sendai, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1977), 25(10), 2692-6
CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 88:50233

AB Acylation of Et 4-bromo-3-hydroxybutanoate with Ac2O, BzCl, diketene, and Ph isocyanate gave Et 3-acetoxy- (I), Et 3-benzoyloxy- (II), Et 3-acetoacetoxy- (III), and Et 3-(N-phenylcarbamoxyloxy)-4-bromobutanoate (IV), resp. Treating I with NaOEt-EtOH gave Et 4-hydroxycrotonate (V) and Et 4-bromocrotonate (VI). II similarly gave VI and Et 4-benzoyloxyacetoxy- (VII). III was converted to V, Et 4-acetoacetoxyacetoxy- (VIII), and 3-acetyl-4-ethoxycarbonylmethyltetrahydrofuran-2-one. Conversely IV under the same conditions gave Et 4-anilinoacetoxy- (IX) instead of the acyl-migrated product.

L9 ANSWER 16 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1964:61218 CAPLUS <<LOGINID::20081229>>
DOCUMENT NUMBER: 60:61218
ORIGINAL REFERENCE NO.: 60:10777g,10778b-d
TITLE: A new synthesis of carnitine
AUTHOR(S): D'Alo, F.; Masserini, A.
CORPORATE SOURCE: Lab. Ric. Vister, Como, Italy
SOURCE: Farmaco, Edizione Scientifica (1964), 19(1), 30-4
CODEN: FRPSAX; ISSN: 0430-0920

DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 60:61218

AB A synthesis of carnitine [DL-β-hydroxy-γ-trimethylaminobutyric acid betaine, (I)] without the use of alkaline cyanide was carried out, beginning with Et γ-bromo-acetoacetate (II). At 5-10°, 209 g. II in 3200 ml. EtOH was added slowly to a solution of 12.65 g. NaBH4 in

25 ml. H₂O, the mixture stirred 4 hrs. at 30°, excess NaBH₄ decomposed with HOAc, the solution evaporated to dryness, taken up in saturated NaCl, and extracted with Et₂O, and the extract dried (Na₂SO₄), evaporated, and distilled in vacuo to give 50% Et γ -bromo- β -hydroxybutyrate (III), b_{0.8} 93-5°.

III (21.1 g.) in 36 g. 33% Me₃N in H₂O was kept 12 hrs. and evaporated in vacuo, the residue in 200 ml. 10% HCl refluxed 3 hrs., the mixture evaporated to dryness in vacuo, and the residue taken up in 60 ml. absolute EtOH; the mixture of carnitine-HBr and -HCl which crystallized was dissolved in H₂O, the solution passed through a column of 300 g. of Amberlite IR-45, and the column washed to a volume of 3 l. The aqueous solution was evaporated to 300 ml. in vacuo and stirred with 30 ml. Amberlite IRA-400 to remove traces of halide ion. After filtration the solution was evaporated to dryness in vacuo at 35°, the residue dissolved in 100 ml. of absolute EtOH, and the solution cooled in brine-ice mixture and precipitated with 250 ml. Me₂CO to give 30% I. In the same manner, γ -amino- β -hydroxybutyric acid (IV), m. 215.5-17.5°, was prepared from III, with 33 ml. concentrated NH₄OH instead of Me₃N. The HCl solution was extracted with Et₂O before refluxing; exchange was carried out on Amberlite IR-45 only, and the halide-free residue was recrystd. from 1:1 EtOH-H₂O. The use of IV as an intermediate in the synthesis of I was not recommended because of the poor yield. Carter and Bhattacharya, CA 49, 3819f.

L9 ANSWER 17 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1930:44129 CAPLUS <<LOGINID::20081229>>

DOCUMENT NUMBER: 24:44129

ORIGINAL REFERENCE NO.: 24:4759a-d

TITLE: Oxidation of unsaturated compounds. II. Preparation and configuration of the 3-halogeno derivatives of crotonic acid

AUTHOR(S): Braun, Geza

SOURCE: Journal of the American Chemical Society (1930), 52, 3167-76

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 24:44129

AB cf. C. A. 23, 817. ClCH₂CH(OH)CH₂CN (I) results in 65% yield by heating 500 g. epichlorohydrin and 145 g. HCN in dilute NaOH at 75-85° for 90 h. or in 25% yield (based on NaCN used) by adding 100 g. NaCN to 300 g. dichlorohydrin in 500 cc. H₂O during 20 min. at 60° and then gradually raising the temperature to 100° during 2 h. I (500 g.) in 260 cc. absolute EtOH and 500 cc. dry Et₂O, saturated with HCl at -15° during 6-8 h., the Et₂O and excess HCl removed, the residue dissolved in 1 l. H₂O and kept at 45-50° for 0.5 h., gives 81% of ClCH₂CH(OH)CH₃CO₃Et, dehydrated by P₂O₆ to 62.5% of a mixture of about 80% of ClCH₃CH:CHCO₃Et and 20% of ClCH:CHCH₂CO₂Et. Saponification of the ester is best carried out with Ba(OH)₂ below 0°; 100 g. of the ester gives 40 g. ClCH₂CH:CHCO₂H (II), m. 83°, and 18 g. of an acid, probably ClCH:CHCH₂CO₃H, m. 2-5° (recrystn. gives 10 g. of the acid, m. 10°). Reduction of the 3,3,3-tri-Cl derivative with Zn in EtOH-AcOH gives 80-85% of the 3,3-di-Cl derivative (III). Details are given for the preparation of dibromohydrin in

54%

yield from C₃H₃(OH)₃, Br and red P; with KCN there results 16.5% of 2-hydroxy-3-bromobutyronitrile, b₂ 117-8°; hydrolysis gives 70% of

Et 2-hydroxy-3-bromobutyrate, b3, 94-6°; P206 gives 28.5% of Et 3-bromocrotonate, b2 80-2°; Ba(OH)3 below 0° 50% of 3-bromocrotonic acid, m. 74°; the saturated aqueous solution contains at room temperature about 3% of acid. The Et ester of II and NaI in Me2CO give Et 3-iodocrotonate b2 90-2° (slight decomposition); it is lachrymatory and causes blisters on the skin; the free acid, yellow, m. 108-8.5° (86% yield), II is catalytically reduced to crotonic acid in about 95% yield; this indicates that II belongs to the crotonic acid series and has the trans-configuration according to Auwers. The reduction of the 3-Br acid proceeds much more slowly and the 3-I acid could not be reduced at all under the conditions used for II. Since the Cl and Br acids can be converted into the I acid, all 3 have the trans-configuration. II is an intermediate product in the reduction of III to crotonic acid.

<http://www.cas.org/support/stngen/stdoc/properties.html>

```
=> e "ethyl 4,4,4-tribromo-3-hydroxybutanoate"/cn
E1      1      ETHYL 4,4'-DICHLOOROBENZILATE/CN
E2      1      ETHYL 4,4'-DIHYDROXYDICOUMARINYL-3,3'-ACETATE/CN
E3      0 -->  ETHYL 4,4,4-TRIBROMO-3-HYDROXYBUTANOATE/CN
E4      1      ETHYL 4,4,4-TRICHLORO-1-BUTENYL CARBONATE/CN
E5      1      ETHYL 4,4,4-TRICHLORO-1-TRIMETHYLSILYLBUTYL CARBONATE/CN
E6      1      ETHYL 4,4,4-TRICHLORO-2-BUTENOATE/CN
E7      1      ETHYL 4,4,4-TRICHLORO-2-CYANO-2-BUTENOATE/CN
E8      1      ETHYL 4,4,4-TRICHLORO-2-CYANOCROTONATE/CN
E9      1      ETHYL 4,4,4-TRICHLORO-3-HYDROXYBUTANOATE/CN
E10     1      ETHYL 4,4,4-TRICHLORO-3-OXOBUTANOATE/CN
E11     1      ETHYL 4,4,4-TRICHLOROACETOACETATE/CN
E12     1      ETHYL 4,4,4-TRICHLOROBUTANOATE/CN

=> e "ethyl 4,4-dibromo-3-hydroxybutanoate"/cn
E1      1      ETHYL 4,4-DIBROMO-2,2-DIETHYL-3-OXOPENTANOATE/CN
E2      1      ETHYL 4,4-DIBROMO-2,2-DIMETHYL-3-OXOBUTANOATE/CN
E3      0 -->  ETHYL 4,4-DIBROMO-3-HYDROXYBUTANOATE/CN
E4      1      ETHYL 4,4-DIBROMOACETOACETATE/CN
E5      1      ETHYL 4,4-DIBUTYL-1-HYDROXY-3-OXO-3,4-DIHYDRO-2-NAPHTHALENEC
                ARBOXYLATE/CN
E6      1      ETHYL 4,4-DICHLORO-3-OXOBUTANOATE/CN
E7      1      ETHYL 4,4-DICYANO-3-METHYL-3-BUTENOATE/CN
E8      1      ETHYL 4,4-DIETHOXY-2-(ETHOXYMETHYLENE)-3-OXOBUTANOATE/CN
E9      1      ETHYL 4,4-DIETHOXY-2-(ETHOXYMETHYLENE)-3-OXOBUTYRATE/CN
E10     1      ETHYL 4,4-DIETHOXY-2-METHYL-1-CYCLOHEXENE-1-CARBOXYLATE/CN
E11     1      ETHYL 4,4-DIETHOXY-3-OXOBUTANOATE/CN
E12     1      ETHYL 4,4-DIETHOXY-3-OXOBUTYRATE/CN
```

```
=> s e2
L10      1 "ETHYL 4,4-DIBROMO-2,2-DIMETHYL-3-OXOBUTANOATE"/CN
```

```
=> d l10 ide
```

```
L10  ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2008 ACS on STN
RN   151556-85-3  REGISTRY
ED   Entered STN:  03 Dec 1993
CN   Butanoic acid, 4,4-dibromo-2,2-dimethyl-3-oxo-, ethyl ester  (CA INDEX
      NAME)
OTHER NAMES:
CN   Ethyl 4,4-dibromo-2,2-dimethyl-3-oxobutanoate
MF   C8 H12 Br2 O3
SR   CA
LC   STN Files:   CA, CAPLUS, CASREACT, CHEMINFORMRX
```

<http://www.cas.org/support/stngen/stdoc/properties.html>

```
=> e "methyl 4,4,4-trifluoro-3-hydroxybutanoate"/cn
E1      1      METHYL 4,4,4-TRIFLUORO-3-AMINO-2-BUTENOATE/CN
E2      1      METHYL 4,4,4-TRIFLUORO-3-HYDROXY-3-(2-MERCAPTO-1,3-THIAZOL-5
-YL) BUTANOATE/CN
E3      1 --> METHYL 4,4,4-TRIFLUORO-3-HYDROXYBUTANOATE/CN
E4      1      METHYL 4,4,4-TRIFLUORO-3-METHOXYBUTANOATE/CN
E5      1      METHYL 4,4,4-TRIFLUORO-3-METHYLTHIOBUTANOATE/CN
E6      1      METHYL 4,4,4-TRIFLUORO-3-OXOBUTANOATE/CN
E7      1      METHYL 4,4,4-TRIFLUOROACETOACETATE/CN
E8      1      METHYL 4,4,4-TRIFLUOROACETYLACETONATE/CN
E9      1      METHYL 4,4,4-TRIFLUOROBUTYNOATE/CN
E10     1      METHYL 4,4,4-TRIFLUOROBUTYRATE/CN
E11     1      METHYL 4,4,4-TRINITROBUTYRATE/CN
E12     1      METHYL 4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,11-HEPTADEC AFLUOR
O-2- IODO-2-METHYLUNDECANOATE/CN
```

```
=> s e3
```

```
L1      1 "METHYL 4,4,4-TRIFLUORO-3-HYDROXYBUTANOATE"/CN
```

```
=> d l1 ide
```

```
L1      ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2008 ACS on STN
RN      475467-53-9  REGISTRY
ED      Entered STN:  09 Dec 2002
CN      Butanoic acid, 4,4,4-trifluoro-3-hydroxy-, methyl ester  (CA INDEX NAME)
OTHER NAMES:
CN      Methyl 4,4,4-trifluoro-3-hydroxybutanoate
MF      C5 H7 F3 O3
SR      CA
LC      STN Files:  CA, CAPLUS, CASREACT, USPAT2
```

/ Structure 19 in file .gra /

****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

```
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
```

```
=> e "methyl 4,4,4-tribromo-3-hydroxybutanoate"/cn
E1      1      METHYL 4,4'-DIMETHOXYBENZILATE/CN
E2      1      METHYL 4,4'-DITHIODIBUTYRATE/CN
E3      0 --> METHYL 4,4,4-TRIBROMO-3-HYDROXYBUTANOATE/CN
E4      1      METHYL 4,4,4-TRICHLORO-3-METHYLBUTANOATE/CN
E5      1      METHYL 4,4,4-TRICHLOROBUTANOATE/CN
E6      1      METHYL 4,4,4-TRICHLOROBUTYRATE/CN
E7      1      METHYL 4,4,4-TRIFLUORO-2-BUTYNOATE/CN
E8      1      METHYL 4,4,4-TRIFLUORO-3-( (B-HYDROXYETHYL) AMINO) -3-( TRI
FLUOROMETHYL) BUTYRATE/CN
E9      1      METHYL 4,4,4-TRIFLUORO-3-( TRIFLUOROMETHYL) CROTONATE/CN
E10     1      METHYL 4,4,4-TRIFLUORO-3-AMINO-2-BUTENOATE/CN
E11     1      METHYL 4,4,4-TRIFLUORO-3-HYDROXY-3-(2-MERCAPTO-1,3-THIAZOL-5
-YL) BUTANOATE/CN
E12     1      METHYL 4,4,4-TRIFLUORO-3-HYDROXYBUTANOATE/CN
```

```
=> e "methyl 4,4,4-trichloro-3-hydroxybutanoate"/cn
E1      1      METHYL 4,4'-DIMETHOXYBENZILATE/CN
```

E2 1 METHYL 4,4'-DITHIODIBUTYRATE/CN
 E3 0 --> METHYL 4,4,4-TRICHLORO-3-HYDROXYBUTANOATE/CN
 E4 1 METHYL 4,4,4-TRICHLORO-3-METHYLBUTANOATE/CN
 E5 1 METHYL 4,4,4-TRICHLOROBUTANOATE/CN
 E6 1 METHYL 4,4,4-TRICHLOROBUTYRATE/CN
 E7 1 METHYL 4,4,4-TRIFLUORO-2-BUTYNOATE/CN
 E8 1 METHYL 4,4,4-TRIFLUORO-3-((B-HYDROXYETHYL)AMINO)-3-(TRIFLUOROMETHYL)BUTYRATE/CN
 E9 1 METHYL 4,4,4-TRIFLUORO-3-(TRIFLUOROMETHYL)CROTONATE/CN
 E10 1 METHYL 4,4,4-TRIFLUORO-3-AMINO-2-BUTENOATE/CN
 E11 1 METHYL 4,4,4-TRIFLUORO-3-HYDROXY-3-(2-MERCAPTO-1,3-THIAZOL-5-YL)BUTANOATE/CN
 E12 1 METHYL 4,4,4-TRIFLUORO-3-HYDROXYBUTANOATE/CN

=> e "ethyl 4,4,4-trichloro-3-hydroxybutanoate"/cn

E1 1 ETHYL 4,4,4-TRICHLORO-2-CYANO-2-BUTENOATE/CN
 E2 1 ETHYL 4,4,4-TRICHLORO-2-CYANOCROTONATE/CN
 E3 1 --> ETHYL 4,4,4-TRICHLORO-3-HYDROXYBUTANOATE/CN
 E4 1 ETHYL 4,4,4-TRICHLORO-3-OXOBUTANOATE/CN
 E5 1 ETHYL 4,4,4-TRICHLOROACETOACETATE/CN
 E6 1 ETHYL 4,4,4-TRICHLOROBUTANOATE/CN
 E7 1 ETHYL 4,4,4-TRICHLOROBUTENOATE/CN
 E8 1 ETHYL 4,4,4-TRICHLOROBUTYRATE/CN
 E9 1 ETHYL 4,4,4-TRIFLUORO-2-((2-HYDROXYETHYL)THIO)-3-OXOBUTANOATE/CN
 E10 1 ETHYL 4,4,4-TRIFLUORO-2-BUTENOATE/CN
 E11 1 ETHYL 4,4,4-TRIFLUORO-2-BUTYNECARBOXYLATE/CN
 E12 1 ETHYL 4,4,4-TRIFLUORO-2-BUTYNOATE/CN

=> s e3

L2 1 "ETHYL 4,4,4-TRICHLORO-3-HYDROXYBUTANOATE"/CN

=> d 12 ide

L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
 RN 19486-93-2 REGISTRY
 ED Entered STN: 16 Nov 1984
 CN Butanoic acid, 4,4,4-trichloro-3-hydroxy-, ethyl ester (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Butyric acid, 4,4,4-trichloro-3-hydroxy-, ethyl ester (6CI, 7CI, 8CI)
 OTHER NAMES:
 CN Ethyl 4,4,4-trichloro-3-hydroxybutanoate
 MF C6 H9 Cl3 O3
 LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS, TOXCENTER, USPAT2, USPATFULL
 (*File contains numerically searchable property data)

L3 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN
 AN 2002:886005 CAPLUS <<LOGINID::20081229>>
 DN 137:369737
 TI Stereoselective hydrogen-transfer process and chiral ruthenium-diamine complex catalyst for producing optically active β -hydroxycarboxylate esters from β -ketocarboxylate esters and hydrogen donors
 IN Tada, Kenichi; Miura, Takashi
 PA Takasago International Corporation, Japan
 SO Eur. Pat. Appl., 9 pp.
 CODEN: EPXXDW
 DT Patent
 LA English
 FAN.CNT 13

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
------------	------	------	-----------------	------

PI	EP 1258470	A2	20021120	EP 2002-291172	20020510
	EP 1258470	A3	20030813		
	EP 1258470	B1	20050817		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2003034665	A	20030207	JP 2002-82865	20020325
	JP 4015450	B2	20071128		
	ES 2247280	T3	20060301	ES 2002-291172	20020510
	US 20030004362	A1	20030102	US 2002-142983	20020513
	US 6723871	B2	20040420		
PRAI	JP 2001-150012	A	20010518		
	JP 2002-82865	A	20020325		

OS CASREACT 137:369737; MARPAT 137:369737

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> e "ethyl 4,4-dichloro-3-hydroxybutanoate"/cn

E1	1	ETHYL 4,4-DIBROMOACETOACETATE/CN
E2	1	ETHYL 4,4-DIBUTYL-1-HYDROXY-3-OXO-3,4-DIHYDRO-2-NAPHTHALENECARBOXYLATE/CN
E3	0 -->	ETHYL 4,4-DICHLORO-3-HYDROXYBUTANOATE/CN
E4	1	ETHYL 4,4-DICHLORO-3-OXOBUTANOATE/CN
E5	1	ETHYL 4,4-DICYANO-3-METHYL-3-BUTENOATE/CN
E6	1	ETHYL 4,4-DIETHOXY-2-(ETHOXYMETHYLENE)-3-OXOBUTANOATE/CN
E7	1	ETHYL 4,4-DIETHOXY-2-(ETHOXYMETHYLENE)-3-OXOBUTYRATE/CN
E8	1	ETHYL 4,4-DIETHOXY-2-METHYL-1-CYCLOHEXENE-1-CARBOXYLATE/CN
E9	1	ETHYL 4,4-DIETHOXY-3-OXOBUTANOATE/CN
E10	1	ETHYL 4,4-DIETHOXY-3-OXOBUTYRATE/CN
E11	1	ETHYL 4,4-DIETHOXY-3-OXOPENTANOATE/CN
E12	1	ETHYL 4,4-DIETHOXYACETOACETATE/CN

=> s e1

L1 1 "ETHYL 4,4-DIBROMOACETOACETATE"/CN

=> d l1 ide

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
 RN 73817-88-6 REGISTRY
 ED Entered STN: 16 Nov 1984
 CN Butanoic acid, 4,4-dibromo-3-oxo-, ethyl ester (CA INDEX NAME)
 OTHER NAMES:
 CN Ethyl 4,4-dibromoacetoacetate
 MF C6 H8 Br2 O3
 LC STN Files: CA, CAPLUS, CASREACT, USPATFULL
<http://www.cas.org/legal/infopolicy.html>

=> s l1

L2 2 L1

=> d l2 ibib abs 1-2

L2 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2003:49611 CAPLUS <<LOGINID::20081229>>
 DOCUMENT NUMBER: 138:237855
 TITLE: Nonselective Bromination-Selective Debromination
 Strategy: Selective Bromination of Unsymmetrical
 Ketones on Singly Activated Carbon against Doubly
 Activated Carbon
 AUTHOR(S): Choi, Han Young; Chi, Dae Yoon

CORPORATE SOURCE: Department of Chemistry, Inha University, Incheon,
402-751, S. Korea
SOURCE: Organic Letters (2003), 5(4), 411-414
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:237855

AB A new synthetic method for the preparation of α -bromo ketones that are brominated in the less activated terminal position of unsym. ketones is reported. Brominations for short reaction times (kinetically controlled) provided internally brominated compds. as the major product. However, brominations for longer reaction times (thermodynamically controlled) gave more of the terminally brominated compound through the reversible reaction by Br₂ and produced hydrogen bromide. Several compds. brominated at the terminal position were successfully prepared through the new synthetic route.

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1980:416984 CAPLUS <<LOGINID::20081229>>

DOCUMENT NUMBER: 93:16984

ORIGINAL REFERENCE NO.: 93:2787a,2790a

TITLE: Carbonylic halides as activators for phototropic compositions

INVENTOR(S): Reardon, Edward Joseph, Jr.; Lipson, Melvin A.

PATENT ASSIGNEE(S): Dynachem Corp., USA

SOURCE: Eur. Pat. Appl., 77 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 5379	A2	19791114	EP 1979-300795	19790509
EP 5379	A3	19791128		
EP 5379	B1	19811223		
EP 5379	B2	19860604		
R: BE, CH, DE, FR, GB, NL, SE				
CA 1153610	A1	19830913	CA 1979-326324	19790425
AU 7946767	A	19791115	AU 1979-46767	19790504
AU 523499	B2	19820729		
JP 54147829	A	19791119	JP 1979-56221	19790508
JP 63052368	B	19881018		
US 4552830	A	19851112	US 1983-555444	19831125
PRIORITY APPLN. INFO.:			US 1978-904144	19780509
			US 1980-195168	A2 19801008
			US 1981-317954	A1 19811103

OTHER SOURCE(S): MARPAT 93:16984

AB Compns., which are useful in the production of resists for use in the electronics industry to manufacture printed circuits, are composed of a polymerizable, curable, or crosslinkable component, a photoinitiator, a color former capable of changing color on contact with a suitable activator, and a latent activator containing an organic halide. The organic halide is a carbonyl compound, such as an aliphatic or cycloaliph. ketone or an ester or amide of a decarboxylic acid. A typical composition for the production of a dry

resist material contains a methacrylic acid-styrene (25:75) copolymer 57.0, trimethylolpropane triacrylate 24.0, tetraethylene glycol diacrylate 12.2, benzophenone 4.0, 4,4'-bis(dimethylamino)benzophenone 0.6, 2-anilino-3-methoxy-6-diethylaminofluoran 0.3, di-Et iodomalate 1.5, benzotriazole 0.4, and MeCOEt 160.0 parts kg weight A dry resist using this composition is used to produce high quality printed circuit boards.

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> e "ethyl 4,4-dichloro-3-hydroxybutanoate"/cn

E1	1	ETHYL 4,4-DIBROMOACETOACETATE/CN
E2	1	ETHYL 4,4-DIBUTYL-1-HYDROXY-3-OXO-3,4-DIHYDRO-2-NAPHTHALENECARBOXYLATE/CN
E3	0 -->	ETHYL 4,4-DICHLORO-3-HYDROXYBUTANOATE/CN
E4	1	ETHYL 4,4-DICHLORO-3-OXOBUTANOATE/CN
E5	1	ETHYL 4,4-DICYANO-3-METHYL-3-BUTENOATE/CN
E6	1	ETHYL 4,4-DIETHOXY-2-(ETHOXYMETHYLENE)-3-OXOBUTANOATE/CN
E7	1	ETHYL 4,4-DIETHOXY-2-(ETHOXYMETHYLENE)-3-OXOBUTYRATE/CN
E8	1	ETHYL 4,4-DIETHOXY-2-METHYL-1-CYCLOHEXENE-1-CARBOXYLATE/CN
E9	1	ETHYL 4,4-DIETHOXY-3-OXOBUTANOATE/CN
E10	1	ETHYL 4,4-DIETHOXY-3-OXOBUTYRATE/CN
E11	1	ETHYL 4,4-DIETHOXY-3-OXOPENTANOATE/CN
E12	1	ETHYL 4,4-DIETHOXYACETOACETATE/CN

=> e "methyl 4,4-dichloro-3-hydroxy-butanoate"/cn

E1	1	METHYL 4,4-DICHLORO-2-IODOBUTYRATE/CN
E2	1	METHYL 4,4-DICHLORO-2-OXO-3-BUTENOATE/CN
E3	0 -->	METHYL 4,4-DICHLORO-3-HYDROXY-BUTANOATE/CN
E4	1	METHYL 4,4-DICHLOROACETOACETATE/CN
E5	1	METHYL 4,4-DICHLOROBUTANOATE/CN
E6	1	METHYL 4,4-DICHLOROBUTYRATE/CN
E7	1	METHYL 4,4-DICYANOBUTYRATE/CN
E8	1	METHYL 4,4-DIETHOXY-1-CYCLOBUTENECARBOXYLATE/CN
E9	1	METHYL 4,4-DIETHOXYBUT-2-YNOATE/CN
E10	1	METHYL 4,4-DIETHOXYCROTONATE/CN
E11	1	METHYL 4,4-DIFERROCENYL PENTANOATE/CN
E12	1	METHYL 4,4-DIFLUORO-2-HEXYNOATE/CN

=> s e2

L3 1 "METHYL 4,4-DICHLORO-2-OXO-3-BUTENOATE"/CN

=> d l3 ide

L3 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
RN 36610-68-1 REGISTRY
ED Entered STN: 16 Nov 1984
CN 3-Butenoic acid, 4,4-difluoro-2-oxo-, methyl ester (CA INDEX NAME)
OTHER NAMES:
CN Methyl 4,4-dichloro-2-oxo-3-butenate
MF C5 H4 F2 O3
LC STN Files: CA, CAPLUS

/ Structure 22 in file .gra /

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

<http://www.cas.org/support/stngen/stndoc/properties.html>

```
=> e "t-butyl 4,4-dichloro-3-hydroxybutanoate"/cn
E1      1      T-BUTYL/CN
E2      1      T-BUTYL 3A-(5-NORBORNENE-2-CARBONYLOXY)-5B-CHOLAN
          -24-OATE-2-HYDROXYETHYL 5-NORBORNENE-2-CARBOXYLATE-MALEIC AN
          HYDRIDE COPOLYMER/CN
E3      0 --> T-BUTYL 4,4-DICHLORO-3-HYDROXYBUTANOATE/CN
E4      1      T-BUTYL 6-TRIFLUOROMETHYL-3-(4-PYRIDINYLAMINO) INDOLE-2-CARBO
          XYLATE/CN
E5      1      T-BUTYL ACRYLATE-DIETHYLENE GLYCOL MONOETHYL ETHER ACRYLATE-
          BUTYL METHACRYLATE-METHYL METHACRYLATE-METHACRYLIC ACID-DI-T
          -BUTYL MALEATE COPOLYMER/CN
E6      1      T-BUTYL ACRYLATE-P-HYDROXYSTYRENE COPOLYMER/CN
E7      1      T-BUTYL ETHYL KETONE/CN
E8      1      T-BUTYL HYDROPEROXIDE/CN
E9      1      T-BUTYL IODIDE/CN
E10     1      T-BUTYL METHACRYLATE-1,3-BUTYLENE GLYCOL DIMETHACRYLATE COPO
          LYMER/CN
E11     1      T-BUTYL METHACRYLATE-DIETHYLENE GLYCOL MONOETHYL ETHER ACRYL
          ATE-2-HYDROXYETHYL METHACRYLATE COPOLYMER/CN
E12     1      T-BUTYL METHACRYLATE-DIETHYLENE GLYCOL MONOETHYL ETHER ACRYL
          ATE-METHACRYLIC ACID COPOLYMER/CN
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```
=> e "propyl 4,4-dichloro-3-hydroxybutanoate"/cn
E1      1      PROPYL 4'-PENTANOYLOXYBIPHENYL-4-CARBOXYLATE/CN
E2      1      PROPYL 4,4-BIS(4-HYDROXYPHENYL) PENTANOATE/CN
E3      0 --> PROPYL 4,4-DICHLORO-3-HYDROXYBUTANOATE/CN
E4      1      PROPYL 4,5-EPOXY-2-HEXENOATE/CN
E5      1      PROPYL 4,6-DIHYDROXY-1,2,3,4-TETRAHYDROISOQUINOLINECARBOXYLA
          TE/CN
E6      1      PROPYL 4,6-DIHYDROXY-2-METHYL-1,2,3,4-TETRAHYDROISOQUINOLINE
          CARBOXYLATE/CN
E7      1      PROPYL 4,8-DIMETHYL-3,4-EPOXYNONANOATE/CN
E8      1      PROPYL 4,8-DIMETHYLNONANOATE/CN
E9      1      PROPYL 4-((2-HYDROXYBENZYL) AMINO) BENZOATE/CN
E10     1      PROPYL 4-((7-(2-FLUORO-4-(METHYLSULFONYL) PHENYL)-6,7-DIHYDRO
          -5H-PYRROLO(2,3-D) PYRIMIDIN-4-YL) OXY)-1-PIPERIDINECARBOXYLAT
          E/CN
E11     1      PROPYL 4-((AMINOSULFONYL) OXY) BENZOATE/CN
E12     1      PROPYL 4-(2-((TERT-BUTYLDIMETHYLSILYL) OXY) ETHYL)-3-FLUOROBEN
          ZOATE/CN
```

```
=> e "4,4-dichloro-3-hydroxybutanoate'/cn
MISMATCHED QUOTE IN EXPAND TERM
Quotation marks (or apostrophes) must be used in pairs,
one before and one after the expression you are setting
off or masking.
```

```
=> e "4,4-dichloro-3-hydroxybutanoate"/cn
E1      1      4,4-DICHLORO-3-BUTENOYL CHLORIDE/CN
E2      1      4,4-DICHLORO-3-HEXANONE/CN
E3      0 --> 4,4-DICHLORO-3-HYDROXYBUTANOATE/CN
E4      1      4,4-DICHLORO-3-METHYL-5-PYRAZOLONE/CN
E5      1      4,4-DICHLORO-3-OXOBUTANOIC ACID/CN
E6      1      4,4-DICHLORO-3-PHENYL-2-CYCLOBUTEN-1-ONE/CN
E7      1      4,4-DICHLORO-3-PHENYL-2-CYCLOBUTENONE/CN
E8      1      4,4-DICHLORO-3-PHENYL-3-BUTEN-2-ONE/CN
E9      1      4,4-DICHLORO-4-SILA-1-DECENE/CN
E10     1      4,4-DICHLORO-4-SILA-1-DOCOSENE/CN
E11     1      4,4-DICHLORO-5,5,5-TRIFLUORO-2-METHYLPENTANOYL CHLORIDE/CN
E12     1      4,4-DICHLORO-5,5,5-TRIFLUOROPENTANOYL BROMIDE/CN
```

```
=> e "phenyl 4,4-dichloro-3-hydroxybutanoate"/cn
E1      1      PHENYL 4,4-BIS(4-HYDROXYPHENYL)PENTANOATE HOMOPOLYMER/CN
E2      1      PHENYL 4,4-DICHLORO-1-BUTANESULFONATE/CN
E3      0 --> PHENYL 4,4-DICHLORO-3-HYDROXYBUTANOATE/CN
E4      1      PHENYL 4,5-DICHLOROISOTHIAZOLE-3-CARBOXYLATE/CN
E5      1      PHENYL 4,5-DIMETHYLSALICYLATE/CN
E6      1      PHENYL 4,5-EPOXY-2-HEXENOATE/CN
E7      1      PHENYL 4,6-DI-O-ACETYL-2,3-DIDEOXY-A-D-ERYTHRO-HEX-2-E
NOPYRANOSIDE/CN
E8      1      PHENYL 4,6-DI-O-ACETYL-2,3-DIDEOXY-B-D-ERYTHRO-HEX-2-EN
OPYRANOSIDE/CN
E9      1      PHENYL 4,6-O-BENZYLIDENE-B-D-GLUCOPYRANOSIDE/CN
E10     1      PHENYL 4,6-O-BENZYLIDENE-1-SELENO-B-D-GLUCOPYRANOSIDE/C
N
E11     1      PHENYL 4,6-O-BENZYLIDENE-2-DEOXY-2-PHTHALIMIDO-1-THIO-B
-D-GLUCOPYRANOSIDE/CN
E12     1      PHENYL 4-(((1R)-1-METHYL-2-((3-METHYLPHENYL)AMINO)-2-OXOETHY
L)OXY)BENZOATE/CN
```

```
=> e "isopropyl 4,4-dichloro-3-hydroxybutanoate"/cn
E1      1      ISOPROPYL 4,4,4-TRIFLUOROACETOACETATE/CN
E2      1      ISOPROPYL 4,4,4-TRIFLUOROBUTYRATE/CN
E3      0 --> ISOPROPYL 4,4-DICHLORO-3-HYDROXYBUTANOATE/CN
E4      1      ISOPROPYL 4,4-DIETHOXYACETOACETATE/CN
E5      1      ISOPROPYL 4,5-DICHLOROPYRIDINE-2-CARBOXYLATE/CN
E6      1      ISOPROPYL 4,5-EPOXY-2-HEXENOATE/CN
E7      1      ISOPROPYL 4,6-DIHYDROXY-2-METHYL-1,2,3,4-TETRAHYDROISOQUINOL
INECARBOXYLATE/CN
E8      1      ISOPROPYL 4,6-DIMETHOXYPYRIMIDINE-2-CARBOXYLATE/CN
E9      1      ISOPROPYL 4-((((2,4-DIMETHOXYPHENYL)AMINO)CARBONYL)OXY)METH
YL)PIPERIDINE-1-CARBOXYLATE/CN
E10     1      ISOPROPYL 4-((((5-TERT-BUTYL-2,3-DIHYDRO-1H-INDEN-1-YL)AMINO
)CARBONYL)AMINO)-1H-INDAZOLE-1-CARBOXYLATE/CN
E11     1      ISOPROPYL 4-((1-(1-(4-CHLOROPHENYL)CYCLOBUTYL)-3-METHYLBUTYL
)AMINO)BUTANOATE/CN
E12     1      ISOPROPYL 4-((4-CHLOROBENZOYL)AMINO)-2-(METHYLTHIO)-1-PHENYL
-1H-IMIDAZOLE-5-CARBOXYLATE/CN
```

```
=> e "ethyl 4,4-dichloro-3-hydroxybutyrate"/cn
E1      1      ETHYL 4,4-DIBROMOACETOACETATE/CN
E2      1      ETHYL 4,4-DIBUTYL-1-HYDROXY-3-OXO-3,4-DIHYDRO-2-NAPHTHALENEC
ARBOXYLATE/CN
E3      0 --> ETHYL 4,4-DICHLORO-3-HYDROXYBUTYRATE/CN
E4      1      ETHYL 4,4-DICHLORO-3-OXOBUTANOATE/CN
E5      1      ETHYL 4,4-DICYANO-3-METHYL-3-BUTENOATE/CN
E6      1      ETHYL 4,4-DIETHOXY-2-(ETHOXYMETHYLENE)-3-OXOBUTANOATE/CN
E7      1      ETHYL 4,4-DIETHOXY-2-(ETHOXYMETHYLENE)-3-OXOBUTYRATE/CN
E8      1      ETHYL 4,4-DIETHOXY-2-METHYL-1-CYCLOHEXENE-1-CARBOXYLATE/CN
E9      1      ETHYL 4,4-DIETHOXY-3-OXOBUTANOATE/CN
E10     1      ETHYL 4,4-DIETHOXY-3-OXOBUTYRATE/CN
E11     1      ETHYL 4,4-DIETHOXY-3-OXOPENTANOATE/CN
E12     1      ETHYL 4,4-DIETHOXYACETOACETATE/CN
```

```
L5      ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2008 ACS on STN
AN      1982:199025  CAPLUS  <<LOGINID::20081229>>
DN      96:199025
OREF    96:32807a,32810a
TI      Alkoxyethynyl ketones
AU      Himbert, G.; Henn, L.
CS      Fachbereich Chem., Kaiserslautern, D-6750, Fed. Rep. Ger.
SO      Organic Preparations and Procedures International (1982), 14(3), 189-94
CODEN:  OPPIAK; ISSN: 0030-4948
```

DT Journal
LA English
OS CASREACT 96:199025

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> s 15

L6 1 L4

=> d 16 all

L6 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
RN 81711-50-4 REGISTRY
ED Entered STN: 16 Nov 1984
CN Butanoic acid, 4,4-dichloro-3-oxo-, methyl ester (CA INDEX NAME)
OTHER NAMES:
CN Methyl 4,4-dichloroacetoacetate
MF C5 H6 Cl2 O3
LC STN Files: CA, CAPLUS, CASREACT
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)

=> s e4

L7 1 "ETHYL 4,4-DIFLUORO-3-OXOBUTANOATE"/CN

=> d 17 ide

L7 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
RN 352-24-9 REGISTRY
ED Entered STN: 16 Nov 1984
CN Butanoic acid, 4,4-difluoro-3-oxo-, ethyl ester (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Acetoacetic acid, 4,4-difluoro-, ethyl ester (6CI, 7CI, 8CI)
OTHER NAMES:
CN 4,4-Difluoro-3-oxobutanoic acid ethyl ester
CN Ethyl 4,4-difluoro-3-oxobutanoate
CN Ethyl 4,4-difluoroacetoacetate
MF C6 H8 F2 O3
CI COM
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX,
CHEMLIST, CSCHEM, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**, NDSL**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> e "ethyl 4,4-dichloro-3-hydroxybutanoate"/cn

E1 1 ETHYL 4,4-DIBROMOACETOACETATE/CN
E2 1 ETHYL 4,4-DIBUTYL-1-HYDROXY-3-OXO-3,4-DIHYDRO-2-NAPHTHALENECARBOXYLATE/CN
E3 0 --> ETHYL 4,4-DICHLORO-3-HYDROXYBUTANOATE/CN
E4 1 ETHYL 4,4-DICHLORO-3-OXOBUTANOATE/CN
E5 1 ETHYL 4,4-DICYANO-3-METHYL-3-BUTENOATE/CN
E6 1 ETHYL 4,4-DIETHOXY-2-(ETHOXYMETHYLENE)-3-OXOBUTANOATE/CN
E7 1 ETHYL 4,4-DIETHOXY-2-(ETHOXYMETHYLENE)-3-OXOBUTYRATE/CN
E8 1 ETHYL 4,4-DIETHOXY-2-METHYL-1-CYCLOHEXENE-1-CARBOXYLATE/CN
E9 1 ETHYL 4,4-DIETHOXY-3-OXOBUTANOATE/CN
E10 1 ETHYL 4,4-DIETHOXY-3-OXOBUTYRATE/CN
E11 1 ETHYL 4,4-DIETHOXY-3-OXOPENTANOATE/CN
E12 1 ETHYL 4,4-DIETHOXYACETOACETATE/CN

=> s e4

L8 1 "ETHYL 4,4-DICHLORO-3-OXOBUTANOATE"/CN

=> d l8 ide

L8 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
RN 6082-74-2 REGISTRY
ED Entered STN: 16 Nov 1984
CN Butanoic acid, 4,4-dichloro-3-oxo-, ethyl ester (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Acetoacetic acid, 4,4-dichloro-, ethyl ester (6CI, 7CI, 8CI)
OTHER NAMES:
CN Ethyl 4,4-dichloro-3-oxobutanoate
MF C6 H8 Cl2 O3
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

=> e "ethyl 4,4-dibromo-3-hydroxybutanoate"/cn

MISMATCHED QUOTE IN EXPAND TERM

Quotation marks (or apostrophes) must be used in pairs,
one before and one after the expression you are setting
off or masking.

=> e "ethyl 4,4-dibromo-3-hydroxybutanoate"/cn

E1 1 ETHYL 4,4-DIBROMO-2,2-DIETHYL-3-OXOPENTANOATE/CN
E2 1 ETHYL 4,4-DIBROMO-2,2-DIMETHYL-3-OXOBUTANOATE/CN
E3 0 --> ETHYL 4,4-DIBROMO-3-HYDROXYBUTANOATE/CN
E4 1 ETHYL 4,4-DIBROMOACETOACETATE/CN
E5 1 ETHYL 4,4-DIBUTYL-1-HYDROXY-3-OXO-3,4-DIHYDRO-2-NAPHTHALENECARBOXYLATE/CN
E6 1 ETHYL 4,4-DICHLORO-3-OXOBUTANOATE/CN
E7 1 ETHYL 4,4-DICYANO-3-METHYL-3-BUTENOATE/CN
E8 1 ETHYL 4,4-DIETHOXY-2-(ETHOXYMETHYLENE)-3-OXOBUTANOATE/CN
E9 1 ETHYL 4,4-DIETHOXY-2-(ETHOXYMETHYLENE)-3-OXOBUTYRATE/CN
E10 1 ETHYL 4,4-DIETHOXY-2-METHYL-1-CYCLOHEXENE-1-CARBOXYLATE/CN
E11 1 ETHYL 4,4-DIETHOXY-3-OXOBUTANOATE/CN
E12 1 ETHYL 4,4-DIETHOXY-3-OXOBUTYRATE/CN

=> s e4

L9 1 "ETHYL 4,4-DIBROMOACETOACETATE"/CN

=> d l9 ide

L9 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
RN 73817-88-6 REGISTRY
ED Entered STN: 16 Nov 1984
CN Butanoic acid, 4,4-dibromo-3-oxo-, ethyl ester (CA INDEX NAME)
OTHER NAMES:
CN Ethyl 4,4-dibromoacetoacetate
MF C6 H8 Br2 O3
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

<http://www.cas.org/legal/infopolicy.html>

=> s l9 and l8 and l7

2 L9

7 L8

50 L7

L10 0 L9 AND L8 AND L7

=> s 17 and 18
50 L7
7 L8
L11 1 L7 AND L8

=> s 17 and 19
50 L7
2 L9
L12 0 L7 AND L9

=> s 18 and 19
7 L8
2 L9
L13 0 L8 AND L9

=> d l11 all

L11 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1959:99446 CAPLUS <<LOGINID::20081229>>
DN 53:99446
OREF 53:17897f-g
ED Entered STN: 22 Apr 2001
TI Study of keto-enol equilibrium. γ -Mono-, di- and trihaloacetoacetic esters
AU Loos, H.; Herman, M.
CS Univ. Ghent
SO Bulletin des Societes Chimiques Belges (1959), 68, 129-38
CODEN: BSCBAG; ISSN: 0037-9646
DT Journal
LA Unavailable
CC 10B (Organic Chemistry: Aliphatic Compounds)
AB ClCH₂CO₂Et (0.5 mole) in Et₂O added as rapidly as possible to 0.5 mole Mg and an excess of FCH₂CO₂Et in an equal volume of Et₂O gave mixture of XCOCH₂CO₂Et (I) (X = CH₂F and = CH₂Cl), separated by distillation Infrared spectra
of pure liquid of I (X = Me, CH₂F, CHF₂, CF₃, CH₂Cl, CHCl₂, and CCl₃ are recorded, and show bands attributed to C:O (ketonic, ketonic ester, and enolic ester), and C:C. Substitution of F for Cl produces larger displacements in wave length and increases in enol content. I (X = CF₃) is nearly completely enolized, while I (X = CCl₃) has a very low enol content, probably due to the steric effect of the Cl atoms.
IT Isomerism
(tautomerism, of Et acetoacetate and its halo derivs.)
IT 141-97-9 609-15-4 1522-41-4 16485-10-2
(Derived from data in the 6th Collective Formula Index (1957-1961))
IT 541-50-4, Acetoacetic acid
(derivs., enolization of)
IT 352-24-9P, Acetoacetic acid, 4,4-difluoro-, ethyl ester
372-31-6P, Acetoacetic acid, 4,4,4-trifluoro-, ethyl ester 372-37-2P, Acetoacetic acid, 4-fluoro-, ethyl ester 638-07-3P, Acetoacetic acid, 4-chloro-, ethyl ester 3702-98-5P, Acetoacetic acid, 4,4,4-trichloro-, ethyl ester 6082-74-2P, Acetoacetic acid, 4,4-dichloro-, ethyl ester
RL: PREP (Preparation)
(preparation of)

=> d l11

L11 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2007:362416 CAPLUS <<LOGINID::20081229>>
DN 148:121227

TI Ruthenium catalyzed asymmetric hydrogenation of α - and
 β -ketoesters in room temperature ionic liquids using chiral P-Phos
ligand
AU Xu, Lijin; Lam, Kim Hung; Ruan, Jiwu; Fan, Qinghua; Chan, Albert S. C.
CS Open Laboratory of Chirotechnology of the Institute of Molecular
Technology for Drug Discovery and Synthesis and Department of Applied
Biology and Chemical Technology, The Hong Kong Polytechnic University,
Hong Kong, Peop. Rep. China
SO ACS Symposium Series (2007), 950(Ionic Liquids in Organic Synthesis),
224-234
CODEN: ACSMC8; ISSN: 0097-6156
PB American Chemical Society
DT Journal
LA English
OS CASREACT 148:121227
RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 3 SEA EXA FUL L15

=> d 117 1-3

L17 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2008 ACS on STN
RN 135548-09-3 REGISTRY
ED Entered STN: 16 Aug 1991
CN Butanoic acid, 4-fluoro-3-hydroxy-, ethyl ester, (S)- (9CI) (CA INDEX
NAME)
FS STEREOSEARCH
MF C6 H11 F O3
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, USPATFULL
(*File contains numerically searchable property data)

L17 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2008 ACS on STN
RN 122666-01-7 REGISTRY
ED Entered STN: 15 Sep 1989
CN Butanoic acid, 4-fluoro-3-hydroxy-, ethyl ester, (R)- (9CI) (CA INDEX
NAME)
FS STEREOSEARCH
MF C6 H11 F O3
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry.

L17 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2008 ACS on STN
RN 122666-01-7 REGISTRY
ED Entered STN: 15 Sep 1989
CN Butanoic acid, 4-fluoro-3-hydroxy-, ethyl ester, (R)- (9CI) (CA INDEX
NAME)
FS STEREOSEARCH
MF C6 H11 F O3
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry.

/ Structure 66 in file .gra /

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L17 ANSWER 3 OF 3 REGISTRY COPYRIGHT 2008 ACS on STN
RN 660-47-9 REGISTRY
ED Entered STN: 16 Nov 1984
CN Butanoic acid, 4-fluoro-3-hydroxy-, ethyl ester (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Butyric acid, 4-fluoro-3-hydroxy-, ethyl ester (7CI, 8CI)
OTHER NAMES:
CN Ethyl γ -fluoro- β -hydroxybutyrate
CN NSC 24564
MF C6 H11 F O3
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, USPATOLD
(*File contains numerically searchable property data)

<http://www.cas.org/legal/infopolicy.html>

=> s l17

L18 6 L17

=> d l18 ibib abs 1-6

L18 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1991:491670 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 115:91670
ORIGINAL REFERENCE NO.: 115:15755a,15758a
TITLE: Optically active fluorine-containing 3-hydroxybutyric acid esters and process for producing same
INVENTOR(S): Tanida, Kaichi; Suzuki, Yoshiichi
PATENT ASSIGNEE(S): Showa Shell Sekiyu K. K., Japan
SOURCE: Eur. Pat. Appl., 7 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 427396	A2	19910515	EP 1990-311017	19901008
EP 427396	A3	19920226		
EP 427396	B1	19940914		
R: DE, FR, GB				
JP 03151348	A	19910627	JP 1989-290346	19891108
US 5118836	A	19920602	US 1990-610748	19901108
PRIORITY APPLN. INFO.:			JP 1989-290346	A 19891108

OTHER SOURCE(S): MARPAT 115:91670

AB Optically active ACH(OH)CH₂CO₂R(I; R = C₃-16 alkyl; A = CF₃, CHF₂, CH₂F) are prepared in high optical purity and without racemization by transesterification of inexpensive and easily available Et esters I (R = Et) with an alc. ROH in the presence of an ammonium salts R₁SO₃- N⁺HR₂R₃R₄ [R₁ = lower alkyl, (un)substituted Ph; R₂-R₄ = lower alkyl, or NR₂R₃R₄ = pyridine] at 80-150° for 8-15 h. Thus, a mixture of 5.0 g (3R)-CF₃CHCOH)CH₂CO₂R₅ (II; R₅ = Et) (prepared by stereoselective reduction of CF₃COCH₂CO₂Et with yeast) 25 mL BuOH, 5.0 g pyridinium toluenesulfonate,

and 25 mL PhMe was refluxed at 110° for 3 h and then solvent was removed over 1 h at 120°. Addnl. PhMe and BuOH were added and the procedure repeated to give, after distillation at 62-69°/3 mmHg, II (R5 = Bu). Similarly II (R5 = octyl, hexyl, heptyl) were prepared

L18 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1989:532606 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 111:132606
ORIGINAL REFERENCE NO.: 111:22187a,22190a
TITLE: Enzymic manufacture of
(R)- γ -substituted- β -hydroxybutyric acid
esters
INVENTOR(S): Yamada, Hideaki; Shimizu, Akira; Miyoshi, Teruzo;
Kato, Masaaki; Morikawa, Tadashi; Hashimoto, Masamichi
PATENT ASSIGNEE(S): Denki Kagaku Kogyo K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63304991	A	19881213	JP 1987-142916	19870608
JP 2566960	B2	19961225		

PRIORITY APPLN. INFO.: JP 1987-142916 19870608

AB Title esters, useful as intermediates for pharmaceuticals and agrochems., are manufactured by treating γ -substituted acetoacetic acid esters with a NADPH-dependent reductase derived from *Sporobolomyces* sp. Thus, a mixture of Et γ -chloroacetoacetate, NADPH, and a reductase from *Sporobolomyces salmonicolor* IFO 1038 was held in a phosphate buffer at pH 6.5 and 28° for 20 h to produce (R)- γ -chloro- β -hydroxybutyric acid Et ester with 98.2% purity and 97% optical purity in 92% yield.

L18 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1989:191289 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 110:191289
ORIGINAL REFERENCE NO.: 110:31739a,31742a
TITLE: Enzymic manufacture of γ -substituted
 β -hydroxybutyrate esters as intermediates for
carnitine synthesis
INVENTOR(S): Yamada, Hideaki; Shimizu, Akira; Miyoshi, Teruzo;
Kato, Masaaki; Morikawa, Tadashi
PATENT ASSIGNEE(S): Denki Kagaku Kogyo K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63309195	A	19881216	JP 1987-145587	19870611
JP 2566962	B2	19961225		

PRIORITY APPLN. INFO.: JP 1987-145587 19870611

AB The title compds., useful as intermediates for carnitine synthesis, are manufactured by treatment of γ -substituted acetoacetate esters with reducing enzymes in aqueous solvents in the presence of organic solvents which

form two phases with H₂O. *Sporobolomyces salmonicolor* IFO 1038 was cultured in a medium containing glucose and corn steep liquor at 28° for 2 days, shake-cultured in the same medium at 28° for 4 days, and centrifuged to collect the bacteria. The bacteria were lysed by sonication in 0.01M phosphate buffer and treated with Et γ -chloroacetoacetate, NADPH, and AcOEt at 30° and pH 8 for 20 h under stirring to produce 92% Et γ -chloro- β -hydroxybutyrate, vs. 52% in the absence of AcOEt.

L18 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1962:38022 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 56:38022
ORIGINAL REFERENCE NO.: 56:7103i,7104f-i,7105a-d
TITLE: Organic fluorine compounds. XX. Some reactions of 1-chloro-3-fluoropropan-2-ol and epifluorohydrin
AUTHOR(S): Bergmann, Ernst D.; Cohen, Sasson; Shahak, Israel
CORPORATE SOURCE: Hebrew Univ., Jerusalem, Israel
SOURCE: Journal of the Chemical Society (1961) 3448-52
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 56:38022

AB cf. CA 55, 9273b.-In 1-chloro-3-fluoropropan-2-ol (I) the Cl atom was much more prone to nucleophilic attack than the F. The reactions with KCN, NaOEt, and NaOPh were studied. Also in epifluorohydrin (II) the oxide ring was opened by diethyl sodiomalonate (III) without attack on the F atom. Alkyl- and arylmagnesium bromide with II gave 1-bromo-3-fluoropropan-2-ol (IV); PhLi gave 1-fluoro-3-phenylpropan-2-ol (V). The preparation of alkyl fluorolactates and fluoropyruvates was described. I (40 g.), 18 g. NaCN, and 10 g. H₂O heated 2 hrs. at 50-60° gave 18 g. γ -fluoro- β -hydroxybutyronitrile (VI), b₁₅ 125-8°. Dry HCl passed 1 hr. through a refluxing solution of 33 g. VI, 33 g. alc., and 3.5 ml. H₂O gave 32 g. Et γ -fluoro- β -hydroxybutyrate (VII), b₁₈ 104-8°. P₂O₅ (10 g.) added portionwise to 16 g. VII in 30 ml. C₆H₆, the mixture refluxed 15 min., and the decantate distilled gave 7 g. Et γ -fluorocrotonate, b₂₁ 66-7°. II (25 g.) refluxed 2 hrs. in 100 ml. 2N alc. NaOEt gave 6 g. 1-ethoxy-3-fluoro-2-propanol (VIII), b₂₈ 71-2°, n_{29D} 1.3995. VIII (31 g.), 41.5 g. Na₂Cr₂O₇, and 70 ml. H₂O treated at 15-20° with 69.5 g. H₂SO₄ and 20 ml. H₂O, the mixture, left 2 hrs., extracted with Et₂O, and distilled gave 18 g. 1-ethoxy-3-fluoroacetone, b₂₅ 63-5°. I (23 g.), 19 g. PhOH, and 8.5 g. NaOH in 70 ml. H₂O refluxed gave 28 g. 1-fluoro-3-phenoxypropan-2-ol (IX), b₄ 110-11°, n_{30D} 1.5138. IX (24 g.) in 70 ml. Me₂CO treated at 15-20° with 15 g. CrO₃, 23 g. concentrated H₂SO₄, and 40 ml. H₂O and the mixture extracted with Et₂O after 3 hrs. gave 17 g. 1-fluoro-3-phenoxyacetone, b₄ 115-17°, n_{28D} 1.5125. II (38 g.) left 2 hrs. at 40-50° with III from 12 g. Na, 250 ml. alc., and 80 g. diethyl malonate, acidified, evaporated, extracted with Et₂O, evaporated, and the residue refluxed 5 hrs. with 100 ml. 10% HCl gave 18 g. δ -fluoro- γ -valerolactone, b₃₂ 127-9°, n_{27D} 1.4260. PhLi (from 4 g. Li) in 100 ml. Et₂O added in 0.5 hr. at -70° to 19 g. II in 50 ml. Et₂O, the temperature raised in 2 hrs. to 0°, and the mixture poured on ice and H₂SO₄ gave 20 g. V, b₁₅ 115-20°. II (14 g.) added dropwise to a Grignard solution (from 2.4 g. Mg and 16 g. PhBr) in 120 ml. Et₂O at 0°, the mixture stirred 1 hr., poured on ice and concentrated H₂SO₄, separated, and distilled gave 7.5 g. IV, b₃₀ 78-80°, and 4.5 g. V. 4-Fluoromethyl-2,2-dimethyl-1,3-dioxolane (67 g.), 80 ml. H₂O, and 20 ml. concentrated HCl heated and stirred to 80-90°, the mixture refluxed

20 min., distilled, the residue diluted with H₂O, warmed 5 hrs. at 60° with 140 ml. 70% HNO₃ and 100 ml. H₂O, left 48 hrs. at room temperature, heated 1 hr. at 60°, and concentrated, gave fluorolactic acid of 90-5% purity. The sirup distilled azeotropically with 50 g. anhydrous alc., 150 ml. C₆H₆, and 0.5 g. p-MeC₆H₄SO₃H and the product distilled gave 31-8 g. Et fluorolactate (X), b₃₀ 96-8°. Similarly, 59 g. Bu fluorolactate was obtained, b₃ 94-5°. Azeotropic condensation of 500 g. glycerol and 430 g. EtCOMe in 500 ml. C₆H₆ in the presence of 20 g. p-MeC₆H₄SO₃H gave 700 g. 2-ethyl-4-hydroxymethyl-2-methyl-1,3-dioxolane (XI), b₂ 72-3°. XI (146 g.) in 100 ml. C₆H₆ added to 24 g. NaH in 600 ml. C₆H₆, the mixture refluxed 0.5 hr., and treated at 25° with 190 g. p-MeC₆H₄SO₂Cl in 300 ml. C₆H₆ gave the p-tosylate as an oil. The tosylate (300 g.) added to 90 g. KF and 300 ml. O(CH₂CH₂OH)₂, the mixture brought slowly to 150°, left at this temperature 5 min., air passed through 10 min., the distillate dissolved in Et₂O, washed, and distilled gave 123 g. 2-ethyl-4-fluoromethyl-2-methyl-1,3-dioxolane, b. 146-7°. X (20.4 g.), 26.7 g. N-bromosuccinimide, and 150 ml. CCl₄ refluxed 1 hr. gave 4.5 g. Et fluoropyruvate (XII), b₂₅ 82-3°. Reaction of XII with 2,4-dinitrophenylhydrazine gave the 2,4-dinitrophenylhydrazone, m. 125-6°, converted at elevated temperature into Et mesoxaldehyde osazone, m. 250° (AcOH). X (20.4 g.), 53.5 g. N-bromosuccinimide, and 250 ml. CCl₄ refluxed 2 hrs. gave 8 g. Et bromofluoropyruvate, b₄₀ 100-1°. With 2,4-dinitrophenylhydrazine this compound gave the above osazone. The infrared spectra were given for a number of the above compds.

L18 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1962:38019 CAPLUS
DOCUMENT NUMBER: 56:38019
ORIGINAL REFERENCE NO.: 56:7104c-e
TITLE: Segregation of organic nitrogen compounds
INVENTOR(S): Fleck, Raymond N.; Wight, Carlyle G.
PATENT ASSIGNEE(S): Union Oil Co.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 2999861		19610912	US 1958-773142	19581112

AB Nonbasic organic N compds. are separated from basic organic N compds. by passage

through a Type X mol. sieve adsorbent. The adsorbents are crystalline Type X zeolitic partially dehydrated metallo alumino silicates having pores of substantially uniform diameter of approx. 7-13 A. (Brit. 777,233). The preferred adsorbent is the 13 A. sodium aluminosilicate 6Na₂O.6Al₂O₃.15SiO₂ "Molecular Sieves 13X." The preferred adsorbent at approx. 265°F. is treated with a 1:1 mixture of hydrocarbons and organic N compds. from a hydrogenated shale oil coker distillate. The N-containing portion of the mixture is approx. 76% (by weight) basic N compds. and 24% nonbasic N compds. After liquid phase treatment 6 hrs., the adsorbent is separated from the raffinate which contains substantially all of the hydrocarbon and some of the N compds. The N-containing portion is approx. 97% (by weight) basic N compds. and 3% nonbasic N compds. The adsorbent is treated with a displacement exchange fluid such as pyridine to give an extract whose N-containing fraction, when separated from pyridine, is approx.

73%

basic N compds. and 27% nonbasic N-compds. Similarly, vapor phase treatment is carried out at about 550°F.

L18 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1962:38018 CAPLUS
DOCUMENT NUMBER: 56:38018
ORIGINAL REFERENCE NO.: 56:7104a-c
TITLE: Diesters
INVENTOR(S): Quaedvlieg, Mathieu; Boehmke, Guenther
PATENT ASSIGNEE(S): Farbenfabriken Bayer A.-G.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1115027		19611012	DE 1958-F25347	19580326

AB Diesters are prepared from dicarboxylic acids with one free OH group. Thus, a surface active polyglycol ether 2000 prepared from 40 moles ethylene oxide and 1 mole diphenyl ethyl phenol is mixed at 80-100° with maleic anhydride 49 dissolved in toluene 100 parts. After 0.5 hr. p-toluenesulfonic acid 5 parts is added to the mixture and the temperature raised to 120-30° to distil the H2O and most of the toluene. The remaining toluene is distilled in vacuo and the p-toluenesulfonic acid neutralized with an equivalent amount of concentrated NaOH. The dicarboxylic acid diester produced is used as a dispersing agent. Similar diesters are prepared from phthalic acid anhydride, succinic acid anhydride, and adipic acid.

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6 L17
44 L13
L19 2 L17 AND L13

=> d 119 ibib abs hitstr

L19 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1989:532606 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 111:132606
ORIGINAL REFERENCE NO.: 111:22187a,22190a
TITLE: Enzymic manufacture of
(R)- γ -substituted- β -hydroxybutyric acid esters
INVENTOR(S): Yamada, Hideaki; Shimizu, Akira; Miyoshi, Teruzo;
Kato, Masaaki; Morikawa, Tadashi; Hashimoto, Masamichi
PATENT ASSIGNEE(S): Denki Kagaku Kogyo K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63304991	A	19881213	JP 1987-142916	19870608
JP 2566960	B2	19961225		

PRIORITY APPLN. INFO.: JP 1987-142916 19870608
AB Title esters, useful as intermediates for pharmaceuticals and agrochems., are manufactured by treating γ -substituted acetoacetic acid esters with a NADPH-dependent reductase derived from Sporobolomyces sp. Thus, a mixture

of Et γ -chloroacetoacetate, NADPH, and a reductase from
Sporobolomyces salmonicolor IFO 1038 was held in a phosphate buffer at pH
6.5 and 28° for 20 h to produce
(R)- γ -chloro- β -hydroxybutyric acid Et ester with 98.2% purity
and 97% optical purity in 92% yield.

IT 95310-94-4P 122666-01-7P

RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP
(Preparation)

(manufacture of, with reductase of Sporobolomyces and NADPH)

RN 95310-94-4 CAPLUS

CN Butanoic acid, 4-bromo-3-hydroxy-, ethyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

/ Structure 68 in file .gra /

RN 122666-01-7 CAPLUS

CN Butanoic acid, 4-fluoro-3-hydroxy-, ethyl ester, (R)- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.

/ Structure 69 in file .gra /

=> d 119 ibib abs hitstr 1-2

L19 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1989:532606 CAPLUS <<LOGINID::20081231>>

DOCUMENT NUMBER: 111:132606

ORIGINAL REFERENCE NO.: 111:22187a,22190a

TITLE: Enzymic manufacture of
(R)- γ -substituted- β -hydroxybutyric acid
esters

INVENTOR(S): Yamada, Hideaki; Shimizu, Akira; Miyoshi, Teruzo;
Kato, Masaaki; Morikawa, Tadashi; Hashimoto, Masamichi

PATENT ASSIGNEE(S): Denki Kagaku Kogyo K. K., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 63304991	A	19881213	JP 1987-142916	19870608
JP 2566960	B2	19961225		

PRIORITY APPLN. INFO.: JP 1987-142916 19870608

AB Title esters, useful as intermediates for pharmaceuticals and agrochems.,
are manufactured by treating γ -substituted acetoacetic acid esters with a
NADPH-dependent reductase derived from Sporobolomyces sp. Thus, a mixture
of Et γ -chloroacetoacetate, NADPH, and a reductase from
Sporobolomyces salmonicolor IFO 1038 was held in a phosphate buffer at pH
6.5 and 28° for 20 h to produce
(R)- γ -chloro- β -hydroxybutyric acid Et ester with 98.2% purity
and 97% optical purity in 92% yield.

IT 95310-94-4P 122666-01-7P

RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP
(Preparation)

(manufacture of, with reductase of Sporobolomyces and NADPH)
RN 95310-94-4 CAPLUS
CN Butanoic acid, 4-bromo-3-hydroxy-, ethyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

/ Structure 70 in file .gra /

RN 122666-01-7 CAPLUS
CN Butanoic acid, 4-fluoro-3-hydroxy-, ethyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 71 in file .gra /

L19 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1989:191289 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 110:191289
ORIGINAL REFERENCE NO.: 110:31739a,31742a
TITLE: Enzymic manufacture of γ -substituted
 β -hydroxybutyrate esters as intermediates for
carnitine synthesis
INVENTOR(S): Yamada, Hideaki; Shimizu, Akira; Miyoshi, Teruzo;
Kato, Masaaki; Morikawa, Tadashi
PATENT ASSIGNEE(S): Denki Kagaku Kogyo K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63309195	A	19881216	JP 1987-145587	19870611
JP 2566962	B2	19961225		

PRIORITY APPLN. INFO.: JP 1987-145587 19870611

AB The title compds., useful as intermediates for carnitine synthesis, are manufactured by treatment of γ -substituted acetoacetate esters with reducing enzymes in aqueous solvents in the presence of organic solvents which form two phases with H₂O. Sporobolomyces salmonicolor IFO 1038 was cultured in a medium containing glucose and corn steep liquor at 28° for 2 days, shake-cultured in the same medium at 28° for 4 days, and centrifuged to collect the bacteria. The bacteria were lysed by sonication in 0.01M phosphate buffer and treated with Et γ -chloroacetoacetate, NADPH, and AcOEt at 30° and pH 8 for 20 h under stirring to produce 92% Et γ -chloro- β -hydroxybutyrate, vs. 52% in the absence of AcOEt.

IT 660-47-9P, Ethyl γ -fluoro- β -hydroxybutyrate
32224-01-4P, Ethyl γ -bromo- β -hydroxybutyrate
RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP (Preparation)

(manufacture of, enzymic, from acetoacetate derivative, two-phase system in)

RN 660-47-9 CAPLUS
CN Butanoic acid, 4-fluoro-3-hydroxy-, ethyl ester (CA INDEX NAME)

/ Structure 72 in file .gra /

RN 32224-01-4 CAPLUS
CN Butanoic acid, 4-bromo-3-hydroxy-, ethyl ester (CA INDEX NAME)

<http://www.cas.org/legal/infopolicy.html>

=> s 133 and 134 and 135
2 L33
38 L34
145 L35
L36 0 L33 AND L34 AND L35

=> s 133 and (or 134) and (or 135)
MISSING TERM 'AND (OR'
The search profile entered contains a left parenthesis,
'(' followed by an operator.

=> s 134 and 135
38 L34
145 L35
L37 5 L34 AND L35

=> d 137 ibib abs ti hit 1-5

L37 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:353051 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 140:374010
TITLE: Preparation of optically active alcohols from ketones
using Daucus carota tuber extract
INVENTOR(S): Yadav, Jhillu Singh; Nanda, Samik; Reddy, Polepally
Thirupathi; Rao, Adari Bhaskar
PATENT ASSIGNEE(S): Council of Scientific and Industrial Research, India
SOURCE: U.S. Pat. Appl. Publ., 11 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 20040082043	A1	20040429	US 2002-282066	20021029
US 7056540	B2	20060606		

PRIORITY APPLN. INFO.: US 2002-282066 20021029

OTHER SOURCE(S): CASREACT 140:374010

AB The present invention relates to an enzymic process for the preparation of optically active chiral alcs. using tuberous root Daucus carota ; particularly invention relates to an enzymic process for the preparation of optically active alcs. by enantioselective reduction of corresponding ketones using tuberous root Daucus carota.

TI Preparation of optically active alcohols from ketones using Daucus carota tuber extract

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

IT 1445-91-6P 1517-67-5P 1572-97-0P, S-1-(4-Methoxyphenyl)-ethanol
4221-99-2P 6033-23-4P 14898-80-7P 16493-60-0P 20107-40-8P
25501-32-0P 26184-62-3P 33401-74-0P 51154-54-2P,
S-1-(4-Methylphenyl)-ethanol 52019-78-0P 53732-47-1P 56816-01-4P
61586-79-6P 85571-85-3P 86728-85-0P 93781-59-0P,
S-1-(4-Hydroxyphenyl)-ethanol 95537-36-3P 96156-72-8P,
S-1-(4-Nitrophenyl)-ethanol 99528-42-4P, S-1-(4-Chlorophenyl)-ethanol
100760-04-1P, S-1-(4-Bromophenyl)-ethanol 101219-73-2P,

S-1-(4-Fluorophenyl)-ethanol 112653-32-4P 120523-15-1P 134625-72-2P
169272-21-3P 169272-22-4P 169272-23-5P 169436-90-2P 297765-54-9P
341513-45-9P 341513-46-0P 438528-24-6P 438528-26-8P

RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP
(Preparation)

(preparation of optically active alcs. from ketones using *Daucus carota*
tuber extract)

L37 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:886005 CAPLUS <<LOGINID::20081231>>

DOCUMENT NUMBER: 137:369737

TITLE: Stereoselective hydrogen-transfer process and chiral
ruthenium-diamine complex catalyst for producing
optically active β -hydroxycarboxylate esters from
 β -ketocarboxylate esters and hydrogen donors

INVENTOR(S): Tada, Kenichi; Miura, Takashi

PATENT ASSIGNEE(S): Takasago International Corporation, Japan

SOURCE: Eur. Pat. Appl., 9 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 13

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1258470	A2	20021120	EP 2002-291172	20020510
EP 1258470	A3	20030813		
EP 1258470	B1	20050817		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003034665	A	20030207	JP 2002-82865	20020325
JP 4015450	B2	20071128		
ES 2247280	T3	20060301	ES 2002-291172	20020510
US 20030004362	A1	20030102	US 2002-142983	20020513
US 6723871	B2	20040420		

PRIORITY APPLN. INFO.: JP 2001-150012 A 20010518
JP 2002-82865 A 20020325

OTHER SOURCE(S): CASREACT 137:369737; MARPAT 137:369737

GI

/ Structure 95 in file .gra /

AB Optically active β -hydroxycarboxylate esters $R_1CH(OH)CH_2CO_2R_2$ [R_1 =
C1-10 (un)branched perfluoroalkyl or perchloroalkyl; R_2 = C1-8 lower
alkyl, (un)substituted benzyl; e.g., optically active Et
4,4,4-trifluoro-3-hydroxybutanoate] are prepared in high yield and
selectivity by stereoselective hydrogen transfer to the corresponding
 β -ketocarboxylate esters $R_1COCH_2CO_2R_2$ (e.g., Et
4,4,4-trifluoro-3-oxobutanoate) in the presence of hydrogen donors (e.g.,
formic acid-triethylamine mixts.) and a chiral ruthenium-diamine complex
catalyst [I; * = asym. carbon atom; R_3, R_4 = alkyl, Ph, (un)substituted
cycloalkyl; R_5 = methanesulfonyl, trifluoromethanesulfonyl,
benzenesulfonyl, (un)substituted naphthyl, camphorsulfonyl,
alkoxycarbonyl, (un)substituted benzoyl; R_6 = H, alkyl; A =
(un)substituted aromatic compound; X = halogen; e.g.,
 $RuCl[(1R,2R)\text{-}p\text{-}TsNHCH(C_6H_5)CH(C_6H_5)NH_2]$ (p-cymene)].

TI Stereoselective hydrogen-transfer process and chiral ruthenium-diamine
complex catalyst for producing optically active β -hydroxycarboxylate

esters from β -ketocarboxylate esters and hydrogen donors
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

IT 372-30-5P, Ethyl 4,4,4-trifluoro-3-hydroxybutanoate
19486-93-2P, Ethyl 4,4,4-trichloro-3-hydroxybutanoate
305322-80-9P, Isopropyl 4,4,4-trifluoro-3-hydroxybutanoate
475467-53-9P, Methyl 4,4,4-trifluoro-3-hydroxybutanoate
475467-55-1P, Methyl 3-hydroxy-4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-
pentadecafluorodecanoate
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective hydrogen-transfer process and chiral ruthenium-diamine
complex catalyst for producing optically active
 β -hydroxycarboxylate esters from β -ketocarboxylate esters and
hydrogen donors)

L37 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:326792 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 137:46794
TITLE: Efficient enantioselective reduction of ketones with
Daucus carota root
AUTHOR(S): Yadav, J. S.; Nanda, S.; Reddy, P. Thirupathi; Rao, A.
Bhaskar
CORPORATE SOURCE: Organic Division, Indian Institute of Chemical
Technology, Hyderabad, 500007, India
SOURCE: Journal of Organic Chemistry (2002), 67(11), 3900-3903
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:46794

AB A novel and efficient reduction of various prochiral ketones such as
acetophenones, α -azido aryl ketones, β -keto esters, and aliphatic
acyclic and cyclic ketones to the corresponding optically active secondary
alcs. with moderate to excellent chemical yield was achieved by using Daucus
carota, root plant cells under extremely mild and environmentally benign
conditions in aqueous medium, has been described. Many of these optically
active alcs. are the potential chiral building blocks for the synthesis of
pharmaceutically important mols. and asym. chiral ligands. Hence, this
biocatalytic approach is found to be the most suitable for the preparation of a
wide range of chiral alcs. and gave inspiration for the development of a
new biotechnol. process.

TI Efficient enantioselective reduction of ketones with Daucus carota root
REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

IT 1445-91-6P 1517-67-5P 1572-97-0P 4221-99-2P 6033-23-4P
14898-80-7P 16493-60-0P 20107-40-8P 25501-32-0P
26184-62-3P 27544-18-9P 33401-74-0P 51154-54-2P 52019-78-0P
53732-47-1P 56816-01-4P 61586-78-5P 61586-79-6P 85571-85-3P
86728-85-0P 93781-59-0P 95537-36-3P 95537-41-0P 96156-72-8P
99528-42-4P 100760-04-1P 101219-73-2P 112653-32-4P 119341-64-9P
120523-15-1P 134625-72-2P 169272-21-3P 169272-22-4P 169272-23-5P
169436-90-2P 297765-54-9P 341513-45-9P 341513-46-0P 438528-24-6P
438528-25-7P 438528-26-8P
RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP
(Preparation)
(enantioselective reduction of ketones with Daucus carota root)

L37 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1991:559159 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 115:159159
ORIGINAL REFERENCE NO.: 115:27255a,27258a

TITLE: Preparation of pyrimidine derivatives as herbicides
 INVENTOR(S): Hatanaka, Masataka; Watanabe, Junichi; Kondo, Yasuo;
 Suzuki, Koichi; Nawamaki, Tsutomu; Watanabe, Shigeomi
 PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 03031266	A	19910212	JP 1989-164942	19890627
PRIORITY APPLN. INFO.:			JP 1989-164942	19890627
OTHER SOURCE(S):	MARPAT 115:159159			

GI

/ Structure 96 in file .gra /

AB Pyrimidine derivs. [I; R = H, (substituted) alkyl, alkali metal ion, alkaline earth metal ion, NH₄, R₁, R₂ = halo, alkyl, alkoxy, haloalkyl, haloalkoxy, dialkylamino; X₁, X₂, Y₁, Y₂ = H, cyano, carboxy, CHO, alkoxycarbonyl, alkoxy, (substituted) alkyl, etc.] are prepared NaH (55% oil) was added to a solution of MeCH(OH)CHMeCO₂Et and sulfone II in THF under cooling and the mixture was stirred at room temperature to give 93% I (R = Et, R₁ = R₂ = MeO,

X1 = Y₁ = H, X₂ = Y₂ = Me), which killed >90% barnyard grass, large crabgrass, etc. at 25.0 g/are.

TI Preparation of pyrimidine derivatives as herbicides

IT 372-30-5P 32328-03-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of herbicide)

IT 105-50-0 383-63-1 1587-15-1 19487-29-7 55107-14-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, in preparation of herbicide)

L37 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1985:184695 CAPLUS <<LOGINID::20081231>>

DOCUMENT NUMBER: 102:184695

ORIGINAL REFERENCE NO.: 102:28965a, 28968a

TITLE: Preparation by yeast reduction and determination of the sense of chirality of enantiomerically pure ethyl (-)-4,4,4-trichloro-3-hydroxy- and (+)-4,4,4-trifluoro-3-hydroxybutanoate

AUTHOR(S): Seebach, Dieter; Renaud, Philippe; Schweizer, W. Bernd; Zueger, Max F.

CORPORATE SOURCE: Lab. Org. Chem., Eidg. Tech. Hochsch., Zurich, CH-8092, Switz.

SOURCE: Helvetica Chimica Acta (1984), 67(7), 1843-53
 CODEN: HCACAV; ISSN: 0018-019X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 102:184695

GI

/ Structure 97 in file .gra /

AB Reduction of EtO₂CCH₂COCR₃ (R = Cl, F) by fermenting baker's yeast (Saccharomyces cerevisiae) on a preparation scale (20-50 g in .apprx.3L H₂O) gave 70-80% EtO₂CCH₂CH(OH)CR₃ (I) with 85% ee (ee = enantiomeric excess) (-)-(S)-I (R = Cl) and 45% ee of (-)-(R)-I (R = F). Recrystn. of I (R = Cl, F) or their 3,5-(O₂N)₂C₆H₃CO₂ esters gave >98% ee. The absolute configurations of I were determined. The x-ray crystal structure of the ester from (+)-(R)-I (R = F) and (-)-camphanoyl chloride, II, was determined.

TI Preparation by yeast reduction and determination of the sense of chirality of enantiomerically pure ethyl (-)-4,4,4-trichloro-3-hydroxy- and (+)-4,4,4-trifluoro-3-hydroxybutanoate

IT 372-30-5P 95605-60-0P 95615-79-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of)

IT 85571-85-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and esterifications of, use of yeast in)

IT 16493-60-0P 16493-64-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, hydrolysis, and esterifications of, use of yeast in)

<http://www.cas.org/legal/infopolicy.html>

=> s l12 and l6

448 L12

88 L6

L13 37 L12 AND L6

=> d l13 ibib abs hitstr 1-5

L13 ANSWER 1 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2008:1383615 CAPLUS <<LOGINID::20081231>>

DOCUMENT NUMBER: 149:512458

TITLE: Enantioselective reduction of ketones

AUTHOR(S): Itsuno, Shinichi

CORPORATE SOURCE: Toyohashi University of Technology, Toyohashi, Japan

SOURCE: Organic Reactions (Hoboken, NJ, United States) (1998),
52, No pp. given

CODEN: ORHNBA

URL: <http://www3.interscience.wiley.com/cgi-bin/mrwhome/107610747/HOME>

PUBLISHER: John Wiley & Sons, Inc.

DOCUMENT TYPE: Journal; General Review; (online computer file)

LANGUAGE: English

OTHER SOURCE(S): CASREACT 149:512458

AB A review of the article Enantioselective reduction of ketones.

IT 86728-93-0P 86728-99-6P 88496-70-2P

90835-93-1P 90866-33-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(Enantioselective Reduction of Ketones)

RN 86728-93-0 CAPLUS

L13 ANSWER 2 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2008:1116154 CAPLUS <<LOGINID::20081231>>

DOCUMENT NUMBER: 149:531428

TITLE: Engineering of NADPH-dependent aldo-keto reductase

from *Penicillium citrinum* by directed evolution to improve thermostability and enantioselectivity
AUTHOR(S): Asako, Hiroyuki; Shimizu, Masatoshi; Itoh, Nobuya
CORPORATE SOURCE: Organic Synthesis Research Laboratory, Sumitomo Chemical Co., Ltd., 1-98, Kasugade-naka 3-chome, Konohana-ku, Osaka, 554-8558, Japan
SOURCE: Applied Microbiology and Biotechnology (2008), 80(5), 805-812
CODEN: AMBIDG; ISSN: 0175-7598
PUBLISHER: Springer
DOCUMENT TYPE: Journal
LANGUAGE: English

AB *Penicillium citrinum* β -keto ester reductase (KER) can catalyze the reduction of Me 4-bromo-3-oxobutyrate (BAM) to Me (S)-4-bromo-3-hydroxybutyrate with high optical purity. To improve the thermostability of KER, protein engineering was performed using error-prone polymerase chain reaction-based random mutagenesis. Variants with the highest levels of thermostability contained the single amino acid substitutions L54Q, K245R, and N271D. The engineered L54Q variant of KER retained 62% of its initial activity after heat treatment at 30°C for 6 h, whereas wild-type KER showed only 15% activity. The L54Q substitution also conferred improved enantioselectivity by KER. An *Escherichia coli* cell biocatalyst that overproduced the L54Q mutant of KER and glucose dehydrogenase as a cofactor regeneration enzyme showed the highest level of BAM reduction in a water/butyl acetate two-phase system.
IT 86728-85-0P, S-Ethyl 4-chloro-3-hydroxybutyrate
88759-56-2P
RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP (Preparation)
(engineering of NADPH-dependent aldo-keto reductase from *Penicillium citrinum* by directed evolution to improve thermostability and enantioselectivity)
RN 86728-85-0 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, ethyl ester, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L13 ANSWER 3 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2008:757902 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 149:221820
TITLE: Asymmetric reduction of substituted α - and β -ketoesters by *Bacillus pumilus* Phe-C3
AUTHOR(S): He, Chunmao; Chang, Dongliang; Zhang, Jie
CORPORATE SOURCE: Guangzhou Institute of Chemistry, Chinese Academy of Sciences, Guangzhou, 510650, Peop. Rep. China
SOURCE: Tetrahedron: Asymmetry (2008), 19(11), 1347-1351
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The enantioselective reduction of substituted α - and β -ketoesters using resting cells of *Bacillus pumilus* Phe-C3 was investigated. Effects of substrate concentration on the catalytic efficiency of the microorganism were studied. Preparative scale productions were carried out under the optimized conditions with 62.4-91.0% yields and 90.2-97.1% ee. The cells retained 80% of initial activity after recycling for six times.
IT 86728-85-0P, Ethyl (S)-4-chloro-3-hydroxybutyrate
95537-36-3P
RL: BPN (Biosynthetic preparation); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)

(asym. reduction of substituted α - and β -ketoesters by *Bacillus pumilus* Phe-C3)
RN 86728-85-0 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, ethyl ester, (3S)- (CA INDEX NAME)

L13 ANSWER 4 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:1101864 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 148:10703
TITLE: A practical and efficient procedure for reduction of carboxylic acids and their derivatives: use of KBH₄-MgCl₂
AUTHOR(S): Qiu, You-Chun; Zhang, Fu-Li; Zhang, Chun-Nian
CORPORATE SOURCE: Pharmacochemistry Division, Shanghai Institute of Pharmaceutical Industry, Shanghai, 200437, Peop. Rep. China
SOURCE: Tetrahedron Letters (2007), 48(43), 7595-7598
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 148:10703

AB The use of KBH₄-MgCl₂ to reduce carboxylic acids and their derivs. to the corresponding alcs. or the resp. reduced products is described. Me (S)-3,4-O-isopropylidene-3,4-dihydroxybutanoate used as a reference substrate was reduced with KBH₄ and MgCl₂ in 1:1 mol ratio to 80 % (S)-1,2-O-isopropylidene-1,2,4-butanetriol. KBH₄-LiCl gave higher yields but LiCl is more expensive than MgCl₂.

IT 86728-85-0, Ethyl (3S)-4-chloro-3-hydroxybutanoate
95537-36-3, Ethyl (3S)-4-bromo-3-hydroxybutanoate
RL: RCT (Reactant); RACT (Reactant or reagent)
(practical and efficient procedure for reduction of carboxylic acids and their derivs. using KBH₄-MgCl₂)

RN 86728-85-0 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, ethyl ester, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L13 ANSWER 5 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:873237 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 147:277913
TITLE: Improved method and kit for automated resolving agents, especially amino acid derivatives, and solvents selection
INVENTOR(S): Vaidya, Niteen A.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 29pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20070185346	A1	20070809	US 2006-347532	20060203
WO 2007092264	A2	20070816	WO 2007-US2800	20070131
WO 2007092264	A3	20071129		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN,

KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK,
 MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO,
 RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT,
 TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
 RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
 IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
 CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
 GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
 KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA
 EP 1981831 A2 20081022 EP 2007-763121 20070131
 R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
 IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR
 PRIORITY APPLN. INFO.: US 2006-347532 A2 20060203
 WO 2007-US2800 W 20070131
 AB The invention is related to a kit for improved identification of the
 optimal conditions for diastereomeric salt crystallization and the selection of
 the optimal resolving agents, especially amino acid derivs., and solvents,
 which
 include A. an array of containers wherein the array is a standard high
 throughput tray and the containers are a multiplicity of substantially
 identical containers or well plates each optionally sealed with a sealant
 or stoppers to avoid loss of chemical solvent; B. wherein each substantially
 identical container has a unique combination of resolving agent in each
 column and at least one suitable solvent in each row; and C. an
 instructional text to use said kit. The tray of 24, 48, 96 or more
 samples is examined simultaneously visually or by standard anal. techniques.
 Resolution of (+)-2-phenylpropionic acid was studied with both amines and
 acids as resolving agents. Strychnine in 96% ethanol was ideal system for
 (+)-isomer, while quinidine in 96% ethanol was the system of choice for
 (-)-isomer. Pyroglutamic acid in 70% isopropanol was ideal system for
 (+)-isomer, while malic acid in 1-butanol was the system of choice for
 (-)-isomer.
 IT 10488-69-4, Ethyl 4-chloro-3-hydroxybutyrate 32224-01-4,
 Ethyl 4-bromo-3-hydroxybutyrate
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (resolving agent; method and kit for automated resolving agents, especially
 from amino acid derivs., and solvents selection)
 RN 10488-69-4 CAPLUS
 CN Butanoic acid, 4-chloro-3-hydroxy-, ethyl ester (CA INDEX NAME)

/ Structure 150 in file .gra /

RN 32224-01-4 CAPLUS
 CN Butanoic acid, 4-bromo-3-hydroxy-, ethyl ester (CA INDEX NAME)

/ Structure 151 in file .gra /

=> d 113 ibib abs hitstr 30-37

L13 ANSWER 30 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1989:532606 CAPLUS <<LOGINID::20081231>>
 DOCUMENT NUMBER: 111:132606
 ORIGINAL REFERENCE NO.: 111:22187a,22190a
 TITLE: Enzymic manufacture of
 (R)- γ -substituted- β -hydroxybutyric acid
 esters
 INVENTOR(S): Yamada, Hideaki; Shimizu, Akira; Miyoshi, Teruzo;

PATENT ASSIGNEE(S): Kato, Masaaki; Morikawa, Tadashi; Hashimoto, Masamichi
 SOURCE: Denki Kagaku Kogyo K. K., Japan
 Jpn. Kokai Tokkyo Koho, 7 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63304991	A	19881213	JP 1987-142916	19870608
JP 2566960	B2	19961225		

PRIORITY APPLN. INFO.: JP 1987-142916 19870608
 AB Title esters, useful as intermediates for pharmaceuticals and agrochems., are manufactured by treating γ -substituted acetoacetic acid esters with a NADPH-dependent reductase derived from *Sporobolomyces* sp. Thus, a mixture of Et γ -chloroacetoacetate, NADPH, and a reductase from *Sporobolomyces salmonicolor* IFO 1038 was held in a phosphate buffer at pH 6.5 and 28° for 20 h to produce (R)- γ -chloro- β -hydroxybutyric acid Et ester with 98.2% purity and 97% optical purity in 92% yield.
 IT 86728-99-6P 88496-70-2P 90866-33-4P 95310-94-4P
 RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP (Preparation)
 (manufacture of, with reductase of *Sporobolomyces* and NADPH)
 RN 86728-99-6 CAPLUS
 CN Butanoic acid, 4-chloro-3-hydroxy-, octyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 152 in file .gra /

RN 88496-70-2 CAPLUS
 CN Butanoic acid, 4-chloro-3-hydroxy-, methyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 153 in file .gra /

RN 90866-33-4 CAPLUS
 CN Butanoic acid, 4-chloro-3-hydroxy-, ethyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

/ Structure 154 in file .gra /

RN 95310-94-4 CAPLUS
 CN Butanoic acid, 4-bromo-3-hydroxy-, ethyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

/ Structure 155 in file .gra /

L13 ANSWER 31 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1989:439010 CAPLUS <<LOGINID::20081231>>
 DOCUMENT NUMBER: 111:39010
 ORIGINAL REFERENCE NO.: 111:6633a,6636a

TITLE: Preparation of β -hydroxyalkanoate esters as synthetic intermediates
 INVENTOR(S): Sayo, Noboru; Akutagawa, Susumu; Saito, Takao; Noyori, Ryoji; Kumobayashi, Hidenori; Takaya, Hidemasa
 PATENT ASSIGNEE(S): Takasago International Corp., Japan
 SOURCE: Eur. Pat. Appl., 12 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
EP 295109	A1	19881214	EP 1988-305293	19880609
EP 295109	B1	19920304		
EP 295109	B2	19960904		
R: CH, DE, FR, GB, LI, NL				
JP 63310847	A	19881219	JP 1987-145975	19870611
JP 06099367	B	19941207		
US 4933482	A	19900612	US 1988-204480	19880609
PRIORITY APPLN. INFO.:			JP 1987-145975	A 19870611
OTHER SOURCE(S):	MARPAT 111:39010			
GI				

/ Structure 156 in file .gra /

AB Optically active R1CHOHCHR3COR2 (R1 = alkyl; CF3, aryl; R2 = alkoxy, alkylthio, PhS, R4R5N where R4,R5 = H, alkyl, PhCH2; R3 = H, halo, alkyl, alkoxy carbonyl, alkoxy carbonylalkyl; R1R3 = to form a 4- to 6-membered alicyclylic) are prepared by asym. hydrogenation of R1COCHR3COR2 in the presence of a ruthenium-optically active phosphine complex. A mixture of MeCOCH2CO2Me, MeOH, H2O, and Ru2Cl4[(+)-I]2(NEt3) (R = H) (preparation given) was autoclaved at 30° and 40kg/cm2 H to give 98% Me (3R)-(-)-3-hydroxybutyrate (99.1% optical purity).
 IT 10488-68-3P 109462-45-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, by hydrogenation of ketocarboxylate)
 RN 10488-68-3 CAPLUS
 CN Butanoic acid, 4-chloro-3-hydroxy-, methyl ester (CA INDEX NAME)

/ Structure 157 in file .gra /

RN 109462-45-5 CAPLUS
 CN Butanoic acid, 4-bromo-3-hydroxy-, methyl ester (CA INDEX NAME)

/ Structure 158 in file .gra /

L13 ANSWER 32 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1989:191289 CAPLUS <<LOGINID::20081231>>
 DOCUMENT NUMBER: 110:191289
 ORIGINAL REFERENCE NO.: 110:31739a,31742a
 TITLE: Enzymic manufacture of γ -substituted β -hydroxybutyrate esters as intermediates for carnitine synthesis
 INVENTOR(S): Yamada, Hideaki; Shimizu, Akira; Miyoshi, Teruzo;

PATENT ASSIGNEE(S): Kato, Masaaki; Morikawa, Tadashi
 SOURCE: Denki Kagaku Kogyo K. K., Japan
 Jpn. Kokai Tokkyo Koho, 8 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63309195	A	19881216	JP 1987-145587	19870611
JP 2566962	B2	19961225		

PRIORITY APPLN. INFO.: JP 1987-145587 19870611

AB The title compds., useful as intermediates for carnitine synthesis, are manufactured by treatment of γ -substituted acetoacetate esters with reducing enzymes in aqueous solvents in the presence of organic solvents which form two phases with H₂O. Sporobolomyces salmonicolor IFO 1038 was cultured in a medium containing glucose and corn steep liquor at 28° for 2 days, shake-cultured in the same medium at 28° for 4 days, and centrifuged to collect the bacteria. The bacteria were lysed by sonication in 0.01M phosphate buffer and treated with Et γ -chloroacetoacetate, NADPH, and AcOEt at 30° and pH 8 for 20 h under stirring to produce 92% Et γ -chloro- β -hydroxybutyrate, vs. 52% in the absence of AcOEt.

IT 10488-68-3P, Methyl γ -chloro- β -hydroxybutyrate
 10488-69-4P, Ethyl γ -chloro- β -hydroxybutyrate
 32224-01-4P, Ethyl γ -bromo- β -hydroxybutyrate
 86728-85-0P, Ethyl (S)- γ -chloro- β -hydroxybutyrate
 90866-33-4P, Ethyl (R)- γ -chloro- β -hydroxybutyrate
 117935-49-6P, Octyl γ -chloro- β -hydroxybutyrate

RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP (Preparation)

(manufacture of, enzymic, from acetoacetate derivative, two-phase system in)

RN 10488-68-3 CAPLUS

CN Butanoic acid, 4-chloro-3-hydroxy-, methyl ester (CA INDEX NAME)

3 ANSWER 33 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1989:6366 CAPLUS <<LOGINID::20081231>>

DOCUMENT NUMBER: 110:6366

ORIGINAL REFERENCE NO.: 110:1195a,1198a

TITLE: Preparation of L-carnitine by microbial reduction of acetoacetic acid derivatives and chemical derivatization

INVENTOR(S): Sih, Charles J.

PATENT ASSIGNEE(S): Sigma-Tau Industrie Farmaceutiche Riunite SpA, Italy

SOURCE: U.S., 11 pp. Cont.-in-part of U.S. Ser. No. 544,957

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4710468	A	19871201	US 1984-580439	19840215
US 4642290	A	19870210	US 1982-447171	19821206
AU 8321758	A	19840614	AU 1983-21758	19831128
AU 566906	B2	19871105		
CA 1225956	A1	19870825	CA 1983-442170	19831129
IL 70352	A	19871020	IL 1983-70352	19831130

FI 8304419	A	19840607	FI 1983-4419	19831202
FI 81115	B	19900531		
FI 81115	C	19900910		
CH 661498	A5	19870731	CH 1983-6448	19831202
DK 8305592	A	19840607	DK 1983-5592	19831205
DK 163917	B	19920421		
DK 163917	C	19920914		
NO 8304461	A	19840607	NO 1983-4461	19831205
NO 159291	B	19880905		
NO 159291	C	19881214		
SE 8306714	A	19840607	SE 1983-6714	19831205
SE 455501	B	19880718		
SE 455501	C	19881110		
GB 2132614	A	19840711	GB 1983-32359	19831205
GB 2132614	B	19860326		
ZA 8309038	A	19840725	ZA 1983-9038	19831205
AT 8304237	A	19910115	AT 1983-4237	19831205
AT 393136	B	19910826		
DE 3344085	A1	19840607	DE 1983-3344085	19831206
DE 3344085	C2	19931014		
FR 2537130	A1	19840608	FR 1983-19505	19831206
FR 2537130	B1	19881014		
NL 8304190	A	19840702	NL 1983-4190	19831206
JP 59118093	A	19840707	JP 1983-230449	19831206
JP 07067674	A	19950314	JP 1993-217710	19930901

PRIORITY APPLN. INFO.:

US 1982-447171 A2 19821206
US 1983-544957 A2 19831021

OTHER SOURCE(S): CASREACT 110:6366; MARPAT 110:6366

AB L-Carnitine is prepared from γ -substituted amides or esters of acetoacetic acid by a stereospecific microbial reduction followed by chemical derivatization steps. γ -Chloroacetoacetic acid octyl ester in Tween 80 was added to an actively growing culture of *Candida kefyr* and incubated for 24 h. The product, 4-chloro-3(R)-hydroxybutyric acid octyl ester (I), was isolated from the broth supernatant in .apprx.70% yield by chromatog. on silica gel. I (1.5 g) was heated with Me₃N in 3 mL EtOH for 2 h to yield a solid that was heated in 10% HCl at 80-90° for 1.5 h. After evaporation of the solvents, 320 mg L-carnitine chloride was extracted

from the residue with EtOH and precipitated with ether.

IT 86728-97-4 86728-98-5 86729-01-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(iodination of)

RN 86728-97-4 CAPLUS

CN Butanoic acid, 4-chloro-3-hydroxy-, hexyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 165 in file .gra /

RN 86728-98-5 CAPLUS

CN Butanoic acid, 4-chloro-3-hydroxy-, heptyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 166 in file .gra /

RN 86729-01-3 CAPLUS

CN Butanoic acid, 4-chloro-3-hydroxy-, decyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 167 in file .gra /

IT 88496-70-2P 90866-33-4P 108100-49-8P

RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP
(Preparation)

(manufacture of, by microbial reduction of acetoacetate, for carnitine
manufacture)

RN 88496-70-2 CAPLUS

CN Butanoic acid, 4-chloro-3-hydroxy-, methyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 168 in file .gra /

RN 90866-33-4 CAPLUS

CN Butanoic acid, 4-chloro-3-hydroxy-, ethyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

/ Structure 169 in file .gra /

RN 108100-49-8 CAPLUS

CN Butanoic acid, 4-chloro-3-hydroxy-, 1,1-dimethylethyl ester, (3R)- (CA
INDEX NAME)

Absolute stereochemistry. Rotation (+).

/ Structure 170 in file .gra /

IT 86728-99-6P 90835-93-1P 90835-94-2P

90835-97-5P 90835-98-6P 91990-59-9P

RL: PREP (Preparation)

(preparation of, microbial, for carnitine manufacture)

RN 86728-99-6 CAPLUS

CN Butanoic acid, 4-chloro-3-hydroxy-, octyl ester, (R)- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.

/ Structure 171 in file .gra /

RN 90835-93-1 CAPLUS

CN Butanoic acid, 4-bromo-3-hydroxy-, octyl ester, (R)- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.

/ Structure 172 in file .gra /

RN 90835-94-2 CAPLUS

CN Butanoic acid, 4-bromo-3-hydroxy-, phenylmethyl ester, (R)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

/ Structure 173 in file .gra /

RN 90835-97-5 CAPLUS

CN Butanoic acid, 4-chloro-3-hydroxy-, propyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 174 in file .gra /

RN 90835-98-6 CAPLUS

CN Butanoic acid, 4-chloro-3-hydroxy-, butyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 175 in file .gra /

RN 91990-59-9 CAPLUS

CN Butanoic acid, 4-chloro-3-hydroxy-, phenylmethyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

/ Structure 176 in file .gra /

L13 ANSWER 34 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1987:596550 CAPLUS <<LOGINID::20081231>>

DOCUMENT NUMBER: 107:196550

ORIGINAL REFERENCE NO.: 107:31521a,31524a

TITLE: Optically active α -halo- β -hydroxybutyrate manufacture by Saccharomyces species

INVENTOR(S): Hasegawa, Masayasu; Okada, Shigetaka; Hamada, Nobutake; Sakai, Kiyofumi; Honda, Hiroshi

PATENT ASSIGNEE(S): Nippon Synthetic Chemical Industry Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 62126997	A	19870609	JP 1985-268811	19851128
US 4933282	A	19900612	US 1986-935199	19861126
PRIORITY APPLN. INFO.:			JP 1985-268811	A 19851128

OTHER SOURCE(S): CASREACT 107:196550

AB γ -Haloacetoacetic acid esters are reacted with a Saccharomyces species to obtain optically active γ -halo- β -hydroxybutyric acid esters. Thus, *S. cerevisiae* IFO 0635 was shake-cultured in YM medium for 48 h. The cells were collected and incubated with a mixture containing 0.8 g glucose and 1 g Et γ -chloroacetoacetate at 27° for 3 h to give Et γ -chloro- β -hydroxybutyrate with .apprx.75% conversion.

IT 10488-69-4P, Ethyl γ -Chloro- β -hydroxybutyrate
109462-45-5P, Methyl γ -Bromo- β -hydroxybutyrate
110930-70-6P, Allyl γ -Chloro- β -hydroxybutyrate
110930-71-7P, Benzyl γ -Chloro- β -hydroxybutyrate
110930-72-8P, Octyl γ -Bromo- β -hydroxybutyrate
RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP (Preparation)
(manufacture of, from haloacetoacetate, by Saccharomyces)

RN 10488-69-4 CAPLUS

CN Butanoic acid, 4-chloro-3-hydroxy-, ethyl ester (CA INDEX NAME)

/ Structure 177 in file .gra /

RN 109462-45-5 CAPLUS
CN Butanoic acid, 4-bromo-3-hydroxy-, methyl ester (CA INDEX NAME)

/ Structure 178 in file .gra /

RN 110930-70-6 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, 2-propen-1-yl ester (CA INDEX NAME)

/ Structure 179 in file .gra /

RN 110930-71-7 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, phenylmethyl ester (CA INDEX NAME)

/ Structure 180 in file .gra /

RN 110930-72-8 CAPLUS
CN Butanoic acid, 4-bromo-3-hydroxy-, octyl ester (CA INDEX NAME)

/ Structure 181 in file .gra /

L13 ANSWER 35 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1987:32369 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 106:32369
ORIGINAL REFERENCE NO.: 106:5415a,5418a
TITLE: Asymmetric reduction of β -keto esters
INVENTOR(S): Ai, Kenzo
PATENT ASSIGNEE(S): Ajinomoto Co., Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 61155354	A	19860715	JP 1984-281337	19841227
PRIORITY APPLN. INFO.:			JP 1984-281337	19841227
AB R1COCH2CO2R2 (R1, R2 = alkyl, alkenyl, alkynyl, aryl, aralkyl, etc.) are asym. reduced in the presence of [R3NR5CHR4(CH2)mY]n (R3, R5 = H, amino-protecting group, R3R5N = heterocycle; R4 = CO2H, CH2OH; m = 0-3; Y = SH, OH, NH2, CO2H when n = 1; Y = S when n = 2) and C1-20 alcs., PhOH, benzyl alc. etc. Thus, LiBH4 was added to a solution of 1.21 mmol (R,R)-N,N'-dibenzoylcystine and 1.61 mmol Me3COH in THF, refluxed, cooled, 1.01 mmol PhCOCH2CO2Et added, and the mixture stirred at -30° to give 94% (R)-(+)-PhCH(OH)CH2CO2Et of 87% optical yield.				
IT 32224-01-4P 90866-33-4P				
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)				
RN 32224-01-4 CAPLUS				
CN Butanoic acid, 4-bromo-3-hydroxy-, ethyl ester (CA INDEX NAME)				

/ Structure 182 in file .gra /

RN 90866-33-4 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, ethyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

/ Structure 183 in file .gra /

L13 ANSWER 36 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1985:130396 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 102:130396
ORIGINAL REFERENCE NO.: 102:20453a,20456a
TITLE: On the steric course of baker's yeast mediated
reduction of alkyl 4-azido- and 4-bromo-3-oxobutyrate.
Synthesis of (R)- and (S)-carnitine
AUTHOR(S): Fuganti, Claudio; Grasselli, Piero; Casati, Paolo;
Carmeno, Massimo
CORPORATE SOURCE: Ist. Chim., Politec. Milano, Milan, 20133, Italy
SOURCE: Tetrahedron Letters (1985), 26(1), 101-4
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 102:130396
AB Bakers' yeast reduction of Et 4-azido- and 4-bromo-3-oxobutyrate affords (3R)
and (3S) carnitines, resp., in high optical purity.
IT 86728-85-0 86728-99-6 95537-36-3
RL: PROC (Process)
(transformation of, by bakers' yeast, stereospecificity in)
RN 86728-85-0 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, ethyl ester, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

/ Structure 184 in file .gra /

RN 86728-99-6 CAPLUS
CN Butanoic acid, 4-chloro-3-hydroxy-, octyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 185 in file .gra /

RN 95537-36-3 CAPLUS
CN Butanoic acid, 4-bromo-3-hydroxy-, ethyl ester, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

/ Structure 186 in file .gra /

L13 ANSWER 37 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1984:437206 CAPLUS <<LOGINID::20081231>>
DOCUMENT NUMBER: 101:37206
ORIGINAL REFERENCE NO.: 101:5813a,5816a
TITLE: L-Carnitine and its intermediate products
INVENTOR(S): Sih, Charles J.
PATENT ASSIGNEE(S): Sigma-Tau Industrie Farmaceutiche Riunite S.p.A.,
Italy
SOURCE: Belg., 38 pp.

DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

CODEN: BEXXAL

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
BE 898396	A1	19840330	BE 1983-212002	19831206
US 4642290	A	19870210	US 1982-447171	19821206
AU 8321758	A	19840614	AU 1983-21758	19831128
AU 566906	B2	19871105		
CA 1225956	A1	19870825	CA 1983-442170	19831129
IL 70352	A	19871020	IL 1983-70352	19831130
FI 8304419	A	19840607	FI 1983-4419	19831202
FI 81115	B	19900531		
FI 81115	C	19900910		
CH 661498	A5	19870731	CH 1983-6448	19831202
DK 8305592	A	19840607	DK 1983-5592	19831205
DK 163917	B	19920421		
DK 163917	C	19920914		
NO 8304461	A	19840607	NO 1983-4461	19831205
NO 159291	B	19880905		
NO 159291	C	19881214		
SE 8306714	A	19840607	SE 1983-6714	19831205
SE 455501	B	19880718		
SE 455501	C	19881110		
GB 2132614	A	19840711	GB 1983-32359	19831205
GB 2132614	B	19860326		
ZA 8309038	A	19840725	ZA 1983-9038	19831205
AT 8304237	A	19910115	AT 1983-4237	19831205
AT 393136	B	19910826		
DE 3344085	A1	19840607	DE 1983-3344085	19831206
DE 3344085	C2	19931014		
FR 2537130	A1	19840608	FR 1983-19505	19831206
FR 2537130	B1	19881014		
NL 8304190	A	19840702	NL 1983-4190	19831206
JP 59118093	A	19840707	JP 1983-230449	19831206
JP 07067674	A	19950314	JP 1993-217710	19930901

PRIORITY APPLN. INFO.:

US 1982-447171 A 19821206
 US 1983-544957 A 19831021

AB L-Carnitine [541-15-1] is prepared from γ -substituted amides or esters of acetoacetic acid by a stereospecific microbial reduction followed by chemical derivatization steps. Thus, γ -chloroacetoacetic acid octyl ester [41051-21-2] in Tween 80 was added to an actively growing culture of Candida kefyr and incubated for 24 h. The product, 4-chloro-3(R)-hydroxybutyric acid octyl ester (I) [86728-99-6], was isolated from the broth supernatant in .apprx.70% yield by chromatog. on silica gel. I (1.5 g) was heated with Me3N [75-50-3] in 3 mL EtOH for 2 h to yield a solid that was heated in 10% HCl at 80-90° for 1.5 h. After evaporation of the solvents, 320 mg L-carnitine chloride [6645-46-1] was extracted from the residue with EtOH and precipitated with ether.

IT 86728-97-4 86728-98-5 86729-01-3

RL: RCT (Reactant); RACT (Reactant or reagent)
 (iodination of)

RN 86728-97-4 CAPLUS

CN Butanoic acid, 4-chloro-3-hydroxy-, hexyl ester, (3R)- (CA INDEX NAME)